

Lattice Hydrogen Transfer in Titanium Hydride Enhances Electrocatalytic Nitrate to Ammonia Conversion

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Supplementary Methods

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Supplementary References

Geometrical coordinates of model structures

Experimental Methods

Characterization

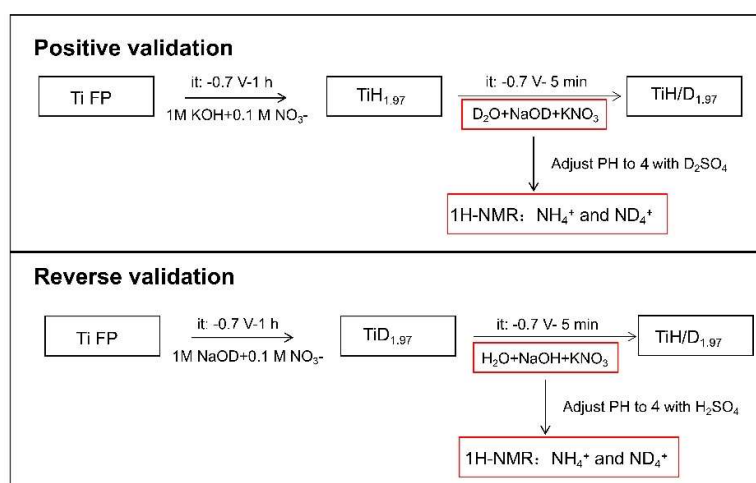
The crystal structure of the prepared electrocatalysts were determined by Smartlabse (RIGAKU) X-ray diffractometer (XRD) with Cu K α radiation ($\lambda=0.15406$ nm). The microstructure and morphology were clarified by Regulus 8100 (HITACHI) Field Emission Scanning Electron Microscope (FESEM) and JEM-2100F (JEOL) transmission electron microscope (TEM) at an acceleration voltage of 200 kV. High-angle annular dark-field scanning TEM (HAADF-STEM) image images were taken on an ARM-200CF (JEOL, Tokyo, Japan) transmission electron microscope, operating at 200 kV, to analyze the microzone structure. A UV-vis spectrophotometer (EVOLUTION 201, Thermo Scientific Corporation) measurements in the range of 200-1000 nm. ^1H -NMR measurements were performed on Bruker AVANCE III HD 600 MHz Nuclear Magnetic Resonance System (NMR-600). X-ray absorption fine structure (XAFS) measurements of the Ti K-edge in transmission mode for Ti foil and titanium hydride powder were performed at Beijing Synchrotron Radiation Facility (BL1W1B station), China.

Isotope labeled active hydrogen transfer in NIRR.

Positive validation method for the participation of lattice hydrogen in hydrogenation reactions in titanium hydride. In an H-type electrolysis cell, a $\text{TiH}_{1.97}/\text{Ti}$ catalyst was prepared. A D_2O solution containing 1 M NaOD and 0.1 M KNO_3 was used as the electrolyte for NIRR. Both the Ti FP and the synthesized $\text{TiH}_{1.97}/\text{Ti}$ electrode were rinsed with D_2O for 10 minutes and dried at 250 °C under argon for 24 h to remove H_2O . NIRR was conducted at -0.7 V vs. RHE for 5 min, after which 10 mL of

electrolyte was taken out and adjusted to pH = 4 with 2 M D₂SO₄, and the resulting products, NH₃ and ND₃, were explored using ¹H NMR.

Reverse validation method for the participation of lattice hydrogen in hydrogenation reactions in titanium hydride. In an H-type electrolysis cell, a TiD_{1.97}/Ti catalyst was prepared by cathodic electrochemical reconstruction for 30 min in a D₂O + NaOD + NO₃⁻ solution. Subsequently, an H₂O solution containing 1 M NaOH and 0.1 M KNO₃ was used as the electrolyte for NIRR. NIRR was conducted at -0.7 V vs. RHE for 5 min, after which 10 mL of electrolyte was taken out and adjusted to pH = 4 with 2 M D₂SO₄, and the resulting products, NH₃ and ND₃, were explored using ¹H NMR. The flow diagram for positive and reverse validation as flow:



Determination of ion concentration

The ultraviolet-visible (UV-Vis) spectrophotometer was used to detect the ion concentration of pre-test and post-test electrolytes after diluting to appropriate concentration to match the range of calibration curves (Fig. S10). The specific detection methods were described as follows.

Determination of ammonia-N

Ammonia-N was determined using salicylic acid-potassium sodium tartrate chromogenic reagent as the color reagent. First, a certain amount of electrolyte was

taken out from the electrolytic cell and diluted to 5 mL to detection range. Next, 0.5 mL salicylic acid-potassium sodium tartrate chromogenic reagent was added and mixed thoroughly, then 0.05 mL sodium nitroprusside and 0.05 mL sodium hypochlorite solution were put into the solution. The absorption intensity at a wavelength of 655 nm was recorded after sitting for 1 h. The concentration-absorbance curve was calibrated using a series of standard ammonium chloride solutions and the ammonium chloride crystal was dried at 105 °C for 2 h in advance.

Determination of nitrate-N

Firstly, a certain amount of electrolyte was taken out from the electrolytic cell and diluted to 5 mL to detection range. Then, 0.1 mL 1 M HCl and 0.01 mL 0.8 wt% sulfamic acid solution were added into the aforementioned solution. The absorption spectrum was measured using an UV-Vis spectrophotometer and the absorption intensities at a wavelength of 220 nm were recorded. The final absorbance value was calculated by this equation: $A = A_{220nm}$. The concentration-absorbance curve was calibrated using a series of standard potassium nitrate solutions and the potassium nitrate crystal was dried at 105-110 °C for 2 h in advance.

Determination of nitrite-N

A mixture of p-aminobenzene sulfonamide (4 g), N-(1-Naphthyl) ethylenediamine dihydrochloride (0.2 g), ultrapure water (50 mL) and phosphoric acid (10 mL, $\rho=1.70$ g mL⁻¹) was used as a color reagent. A certain amount of electrolyte was taken out from the electrolytic cell and diluted to 10 mL to detection range. Next, 0.1 mL color reagent was added into the aforementioned 10 mL solution and mixed uniformly, and the absorption intensity at a wavelength of 540 nm was recorded after sitting for 20 min. The concentration-absorbance curve was calibrated using a series of standard sodium nitrite solutions.

Isotope Labeling Experiments.

99.21% K^{15}NO_3 was used as the feeding N-source to perform the isotopic labeling nitrate reduction experiments to clarify the source of ammonia. 1 M KOH was used as electrolyte and K^{15}NO_3 with a concentration of 0.1 M $^{15}\text{NO}_3^-$ - ^{15}N was added into the cathode compartment as the reactant. After electroreduction, electrolyte with obtained $^{15}\text{NH}_4^+$ - ^{15}N was taken out and the pH value was adjusted to be weak acid with 2 M H_2SO_4 for further analysis by ^1H NMR (600 MHz) with external standards of maleic acid.

Computational details

All the spin-polarized density functional theory calculations were performed by using the Vienna ab initio Simulation Program (VASP)^{1, 2}. The generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) form and a cutoff energy of 500 eV for planewave basis set were adopted³. A $3 \times 3 \times 1$ Monkhorst-Pack grid was used for sampling the Brillouin zones at structure optimization⁴. The ion-electron interactions were described by the projector augmented wave (PAW) method⁵. A Gaussian smearing of 0.05 eV to the orbital occupation was applied during the geometry optimization and for the total energy computations. The convergence criteria of structure optimization were choose as the maximum force on each atom less than $0.02 \text{ eV}/\text{\AA}$ with an energy change less than $1 \times 10^{-5} \text{ eV}$. Periodic slabs with 2×3 and 2×2 supercell were applied to model the catalyst surfaces, respectively, and a sufficient vacuum of 18 \AA was considered in the orthogonal direction to avoid periodic interaction. The DFT-D3 semiempirical correction was described via Grimme's scheme method⁶. According to previously reports, the effective strength parameter ($U_{eff} = U - J$) of the Hubbard on-site Coulomb correlation were set at 2.58 eV for Ti element⁷.

The implicit solvent model (VASPsol) was adopted since the reaction normally takes place in an aqueous solution⁸. To calculate the kinetic energy barrier of chemical reactions, the climbing image nudged elastic band (CI-NEB) method with 6 images was used to search for the transition states (vibrational frequencies were evaluated to confirm minima and transition states), in which all of the force components perpendicular to the tangent of the reaction path were relaxed to be less than 0.05 eV/Å⁹.

The Gibbs free energy change (ΔG) for each elemental step is defined as^{10, 11}:

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S + \Delta G_U + \Delta G_{pH} \quad (1)$$

where ΔE and ΔZPE are the adsorption energy based on density functional theory calculations and the zero-point energy correction, respectively. T , ΔS , U , and ΔG_{pH} represent the temperature ($T = 298$ K), the entropy change, the applied electrode potential, and the free energy correction of the pH ($pH = 0$), respectively. In addition, the atomic coordinates of the optimized computational models had been provided as a separate supporting file named as supplementary data 1.

Supplementary Figures

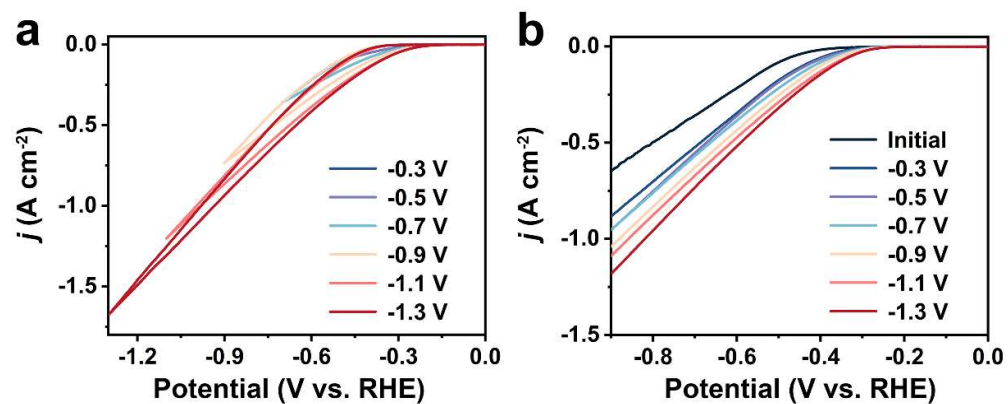


Fig. S1 (a) Cyclic voltammograms within the different range from 0 V to -1.3 V vs.

RHE. **(b)** Corresponding polarization curves after **(a)**. (without iR compensation)

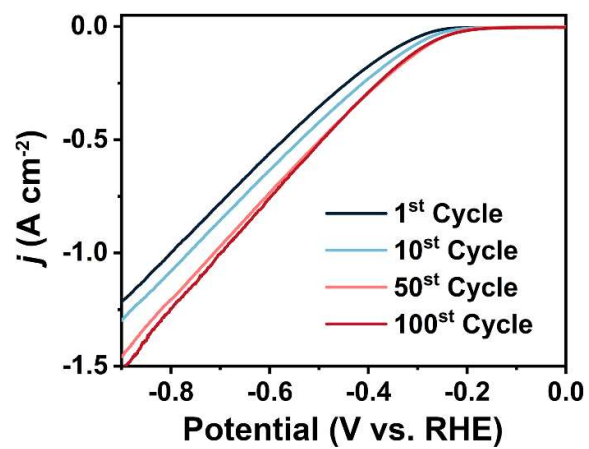


Fig. S2 Corresponding polarization curves after Cyclic voltammograms of different cycles from -1.3 V vs. RHE. (without iR compensation)



Ti FP



TiH_{1.97}/Ti

Fig. S3 The digital images of Ti FP and TiH_{1.97}/Ti.

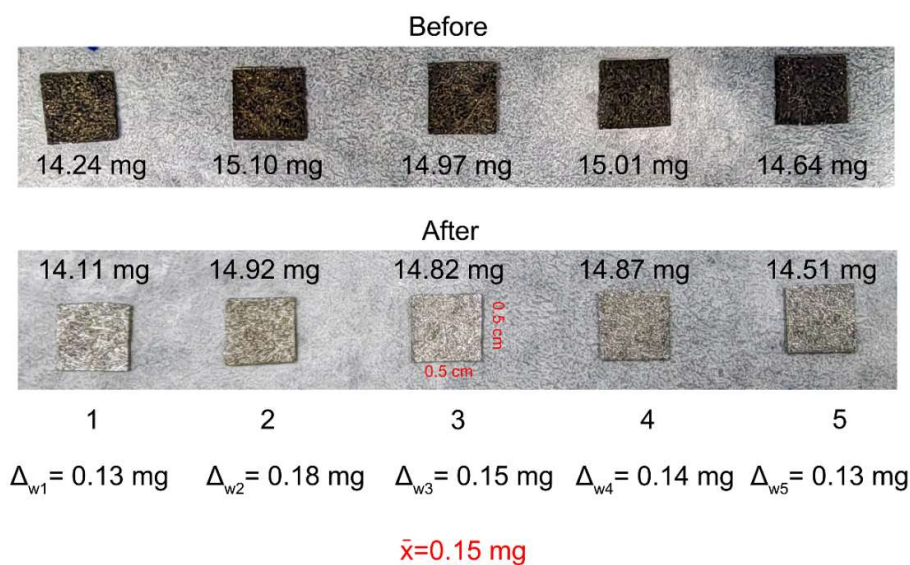


Fig. S4 Weighing the difference in mass before and after the reaction with 0.1 M HCl.

Note: We used the strong oxidizing agent (HCl: 0.1 M) to undergo a chemical reaction with the electrode ($\text{TiH}_{1.97}/\text{Ti}$). By weighing the difference in mass before and after the reaction (Fig. S4), we could obtain the weight of the titanium hydride loaded on the electrode (data from five sets of measurements were taken and the average was calculated). This was because metal hydrides are highly reactive with hydrochloric acid, while metallic titanium did not react with HCl, so the weight loss on the electrode belongs to titanium hydride. Through calculation, we obtained a titanium hydride loading of 0.6 mg cm^{-2} on the electrodes.

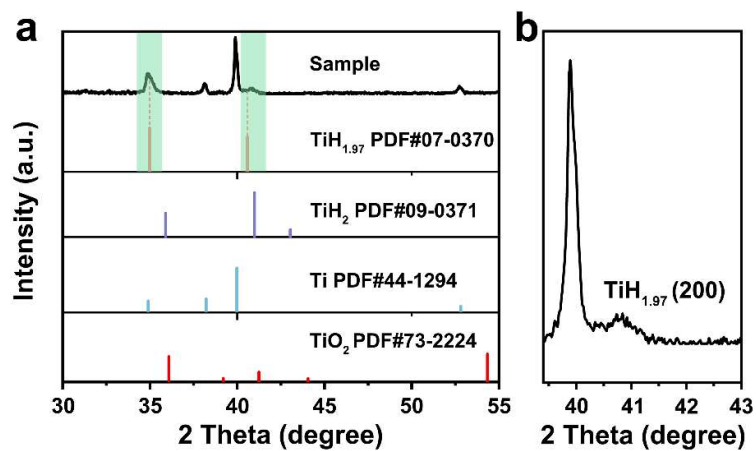


Fig. S5 (a) The XRD spectrum for electrode and the standard spectra of Ti (PDF#44-1294), TiO₂ (PDF#73-2224), TiH₂ (PDF#09-0371) and TiH_{1.97} (PDF#07-0370) and **(b)** the magnified local image of the characteristic peak corresponding to TiH_{1.97} (200).

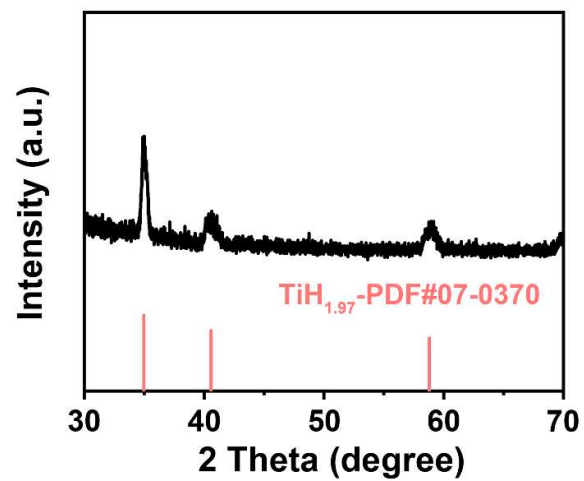


Fig. S6 A separate XRD test of the TiH_{1.97} on the electrode surface.

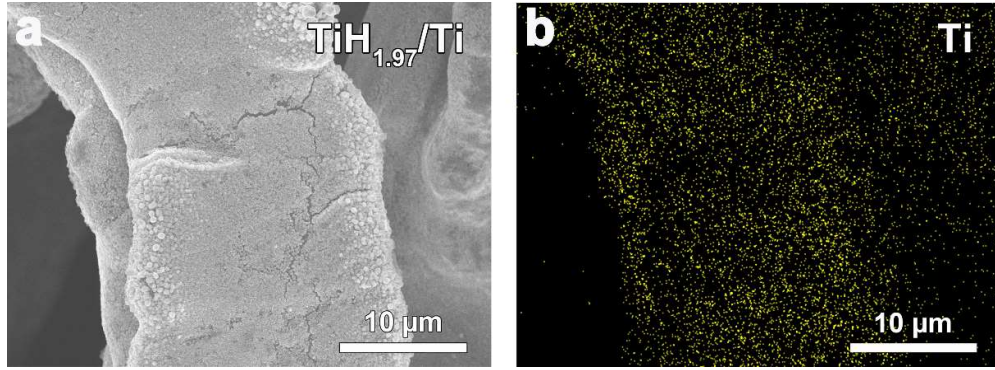


Fig. S7 EDX mappings of titanium hydride.

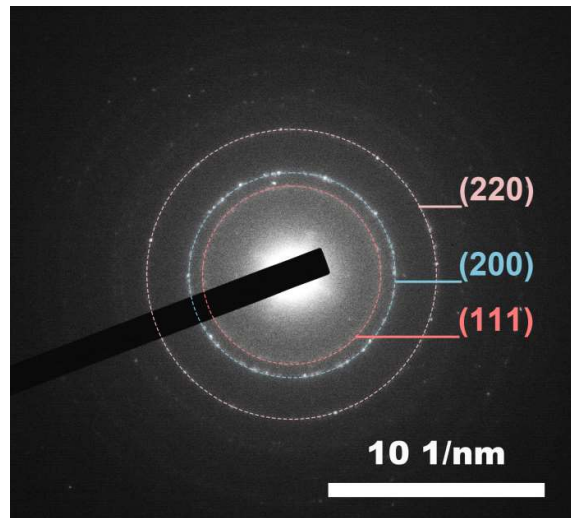


Fig. S8 SAED pattern of the titanium hydride.

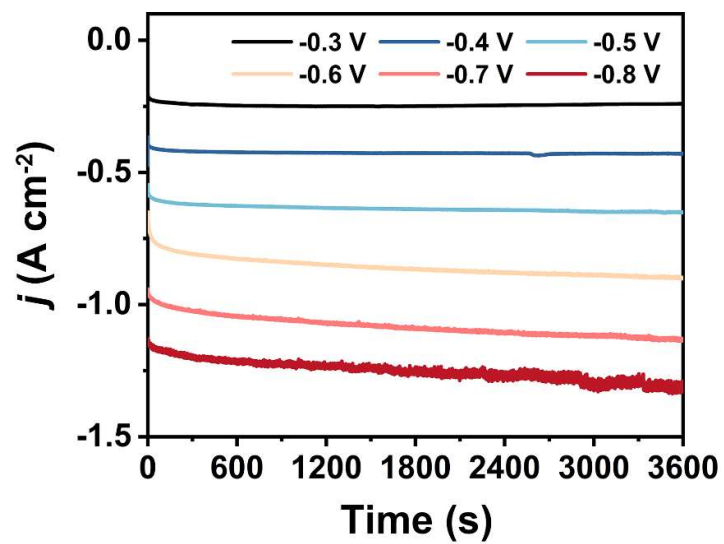


Fig. S9 i-t curves of the titanium hydride catalyst against various work potentials obtained in NO_3^- electrolyte after the NIRr test. (without iR compensation)

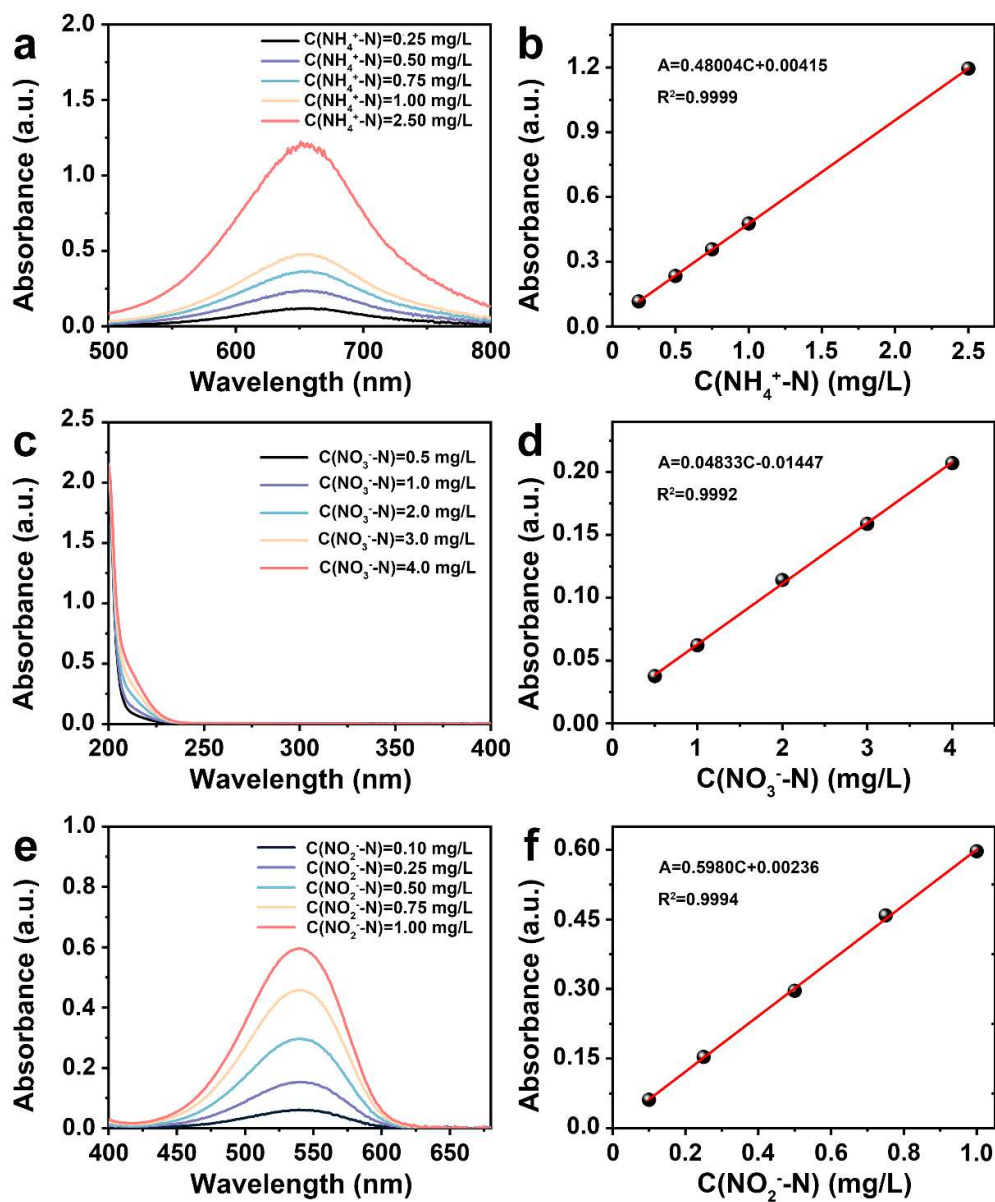


Fig. S10 Plotting of standard curves of (a, b) $\text{NH}_4^+\text{-N}$, (c, d) $\text{NO}_3^-\text{-N}$ and (e, f) $\text{NO}_2^-\text{-N}$

N The calibration curves all show good linearity.

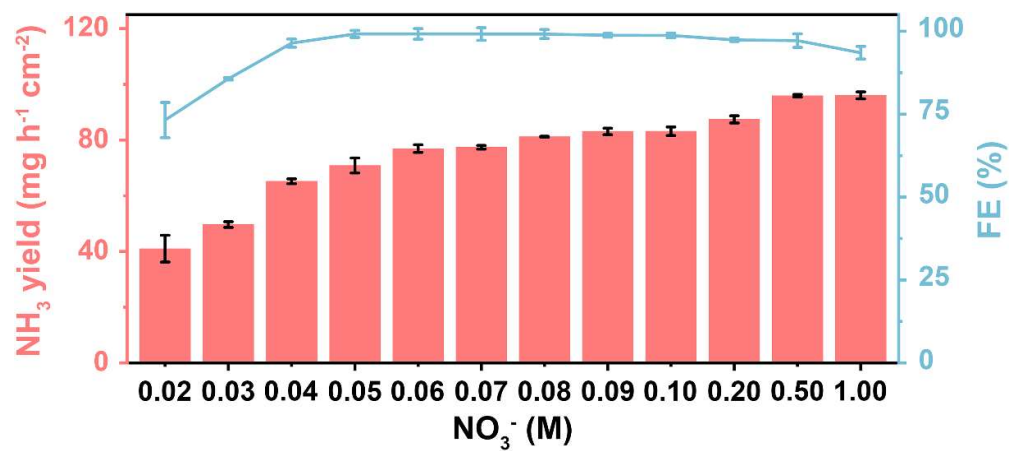


Fig. S11 NH_3 yield and FE for titanium hydride at NO_3^- concentration of 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.10, 0.20, 0.50 and 1.00 M. The NH_3 yield and FE are calculated once per hour. Error bars indicate their relative standard deviations of the mean ($n=3$).

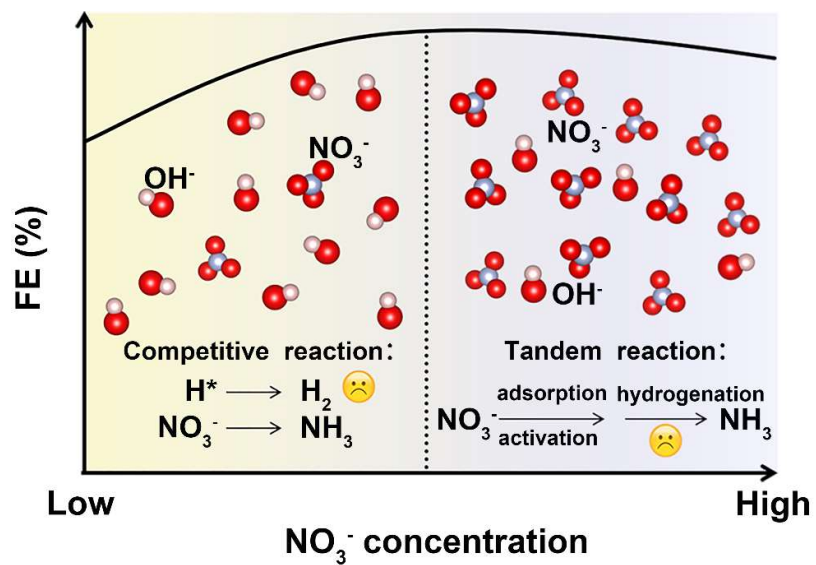


Fig. S12 The schematic diagram of the effect of NO_3^- concentration on FE. The light purple, red and pink spheres represent N, O, and H atoms, respectively.

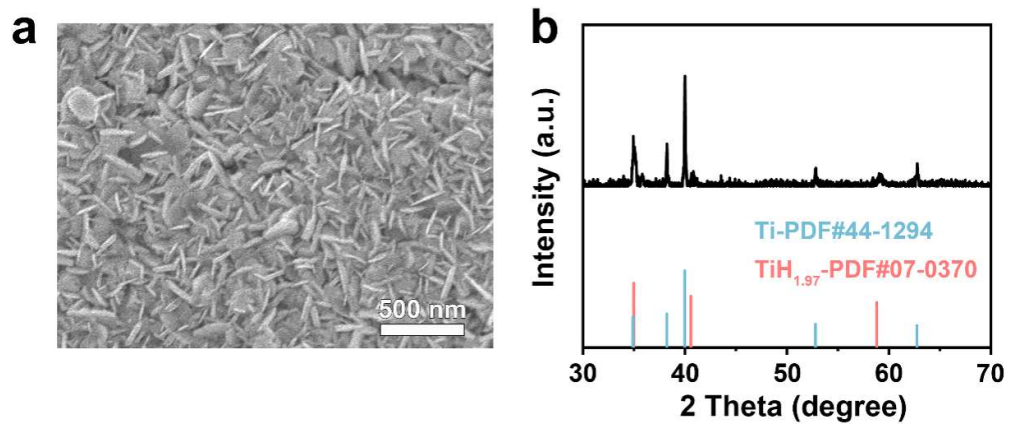


Fig. S13 (a) SEM image and **(b)** XRD patterns of titanium hydride after stability testing.

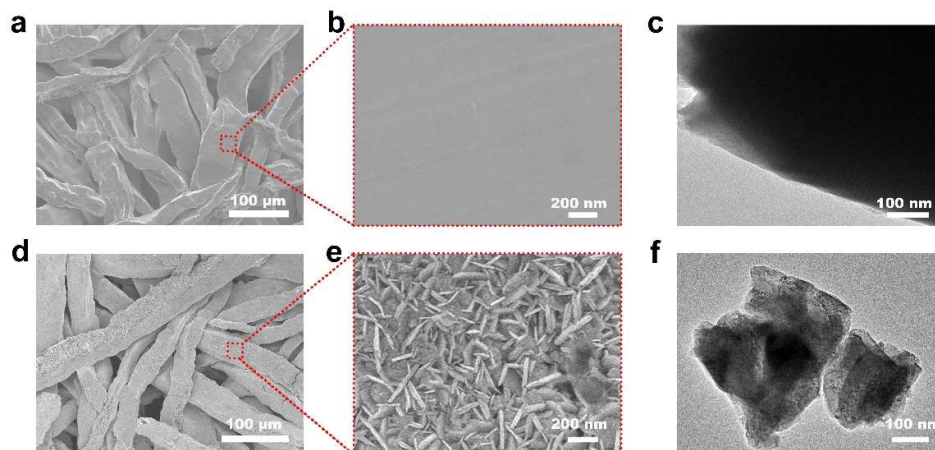


Fig. S14 (a, b) SEM and **(c)** TEM images of the original Ti FP. **(d, e)** SEM and **(f)** TEM images of the titanium hydride after electrocatalysis.

Note: Based on the SEM images in Fig. S14a and the locally magnified image (Fig. S14b), it could be seen that the Ti FP were formed by the intertwined and interwoven titanium fibers, and the diameter of a single titanium fiber was approximately 60 μm. The surface of the titanium fibers was smooth and free of any impurities. The TEM image (Fig. S14c) also showed the smooth surface and solid structure of the titanium fibers. After NIRR treatment, $\text{TiH}_{1.97}/\text{Ti}$ still maintained the mesh-like structure of the titanium fiber paper (Fig. S14d), and the titanium hydride nanosheets on the surface did not undergo significant morphological changes compared to the pre-electrocatalysis (Fig. S14e and Fig. 1g). The TEM image (Fig. S14f) also showed that the surface of the nanosheets remained smooth after electrochemical catalysis, further indicating the good structural stability of the catalyst.

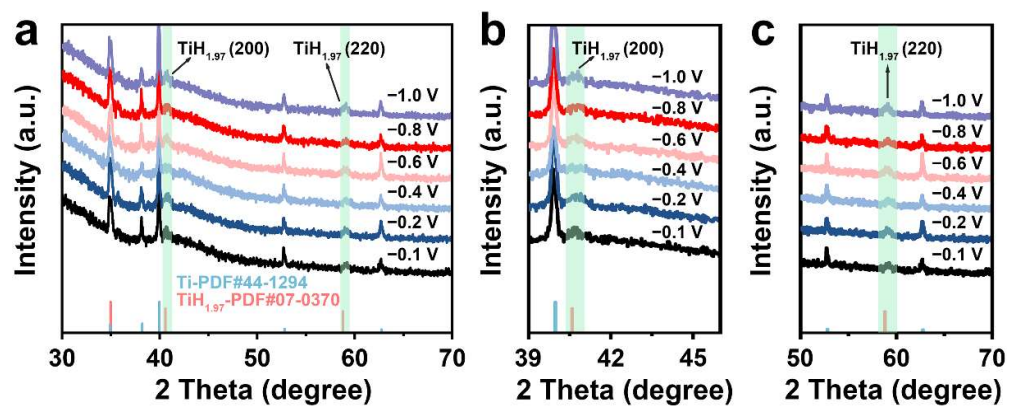


Fig. S15 (a) XRD spectrum of electrode during NIRR at applied potentials of -0.1 , -0.2 , -0.4 , -0.6 , -0.8 and -1.0 V vs. RHE. The magnified local image of the characteristic peak corresponding to (b) $\text{TiH}_{1.97}(200)$ and (c) $\text{TiH}_{1.97}(220)$.

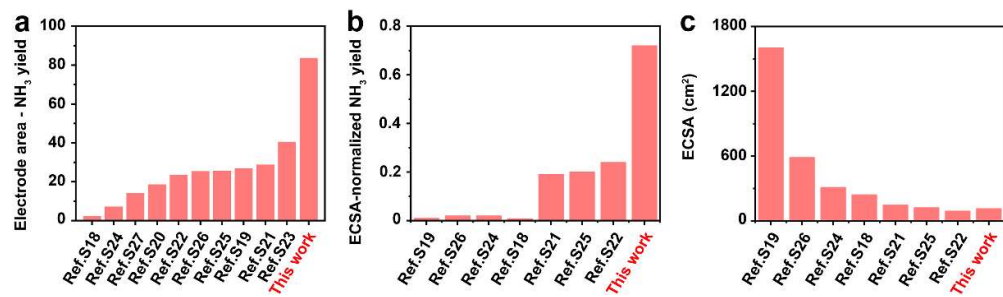


Fig. S16 Comparison of the (a) Electrode area - NH₃ yield (mg h⁻¹ cm⁻²), (b) ECSA-normalized NH₃ yield and (c) ECSA with other literatures.

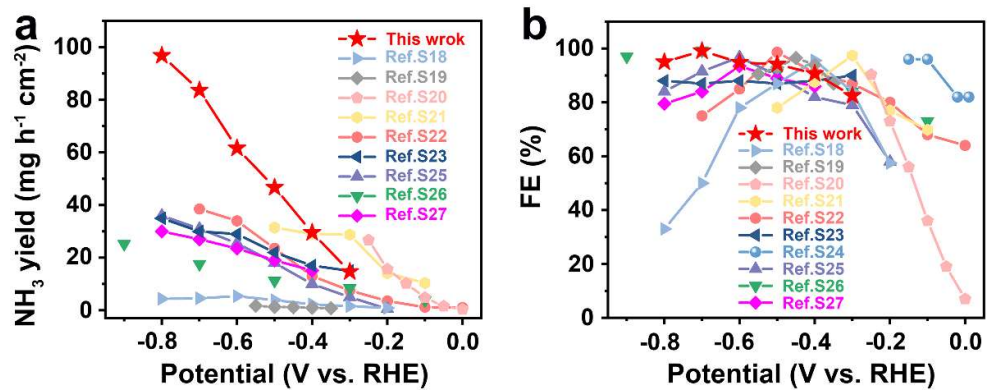


Fig. S17 The comparison of **(a)** NH₃ yields and **(b)** FE under different voltages with other literature. (without iR compensation)

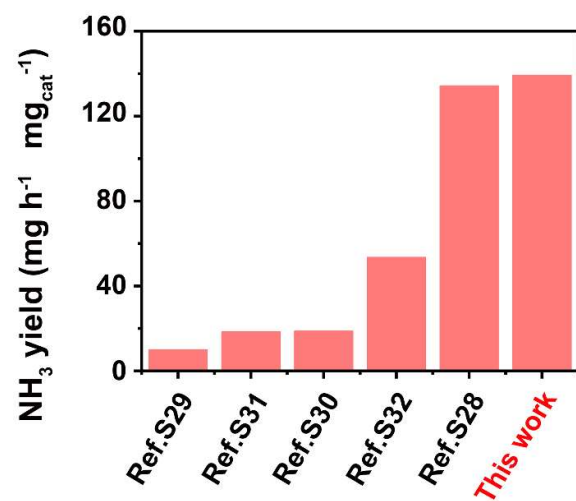


Fig. S18 Comparison of the NH₃ yield with other literature by weight of titanium hydride powder.

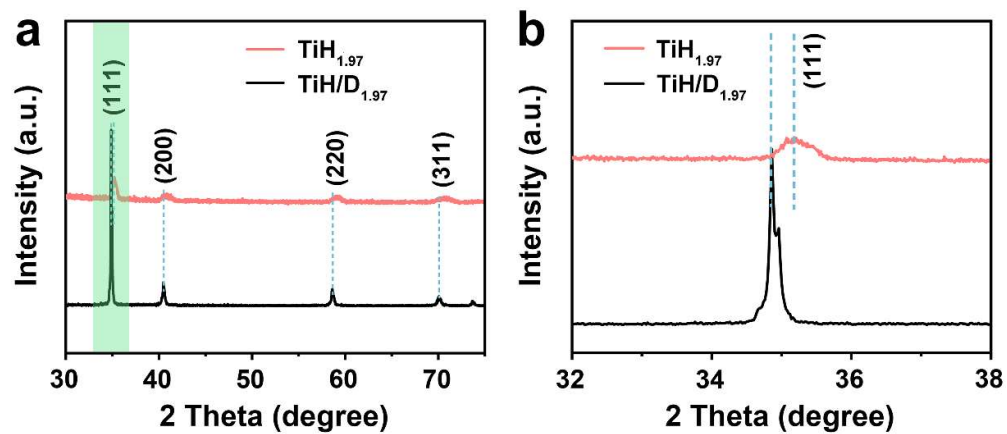


Fig. S19 (a) XRD spectrum of electrode before and after the isotope tracking experiments. **(b)** The local amplification of the characteristic peaks corresponding to the (111) lattice plane.

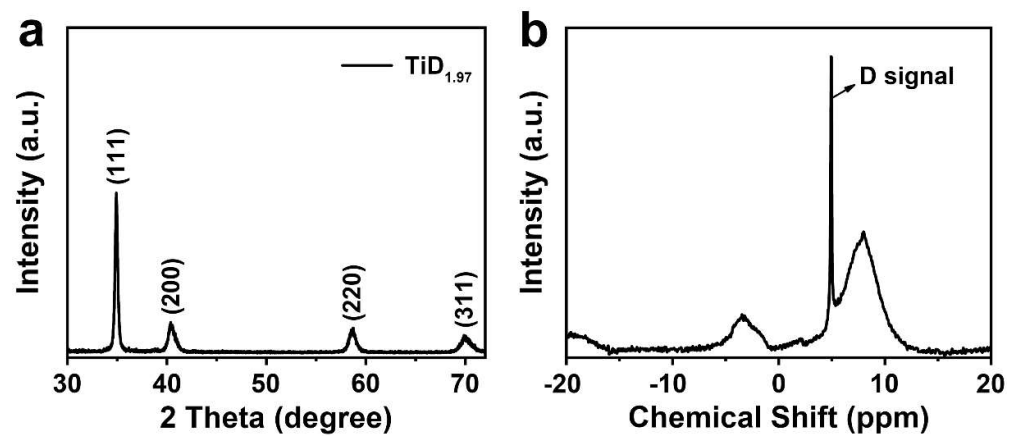


Fig. S20 (a) XRD and (b) solid-state NMR spectra for $\text{TiD}_{1.97}$.

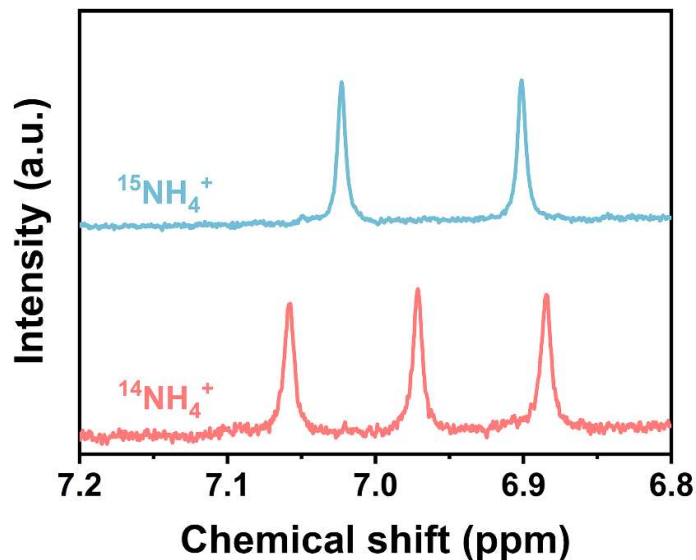


Fig. S21 ¹H NMR spectra of the electrolyte after the NIRR using ¹⁵NO₃⁻ as the feedstock.

Note: To confirm that the isotopic labeling experiments were conducted using ¹⁵NO₃⁻ and ¹⁴NO₃⁻ as reactants, respectively. The ¹⁵NH₃ signal, a classic marker, was detected at $\delta = 6.90$ and 7.02 ppm in the ¹H nuclear magnetic resonance (NMR) spectrum with ¹⁵NO₃⁻ as the feedstock (Fig. S21), showing no difference compared to the ¹H NMR spectrum of (¹⁵NH₄)₂SO₄. Similarly, using ¹⁴NO₃⁻ as the reactant in the electrolyte yielded consistent detection results with that of (¹⁴NH₄)₂SO₄ via ¹H NMR analysis, illustrating that the NH₃ was generated entirely by NIRR¹².

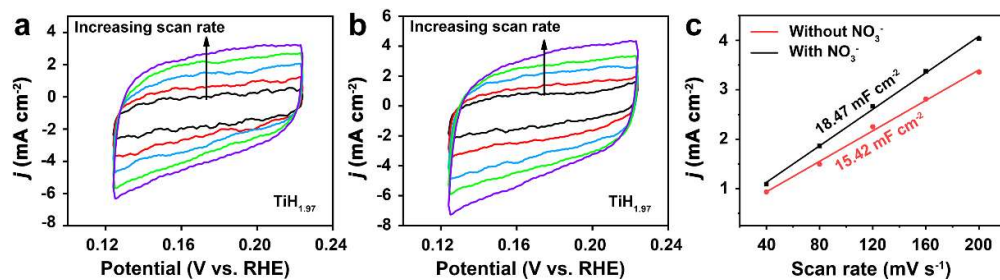


Fig. S22 CV curves of (a) Titanium hydride in 1 M KOH. (b) Titanium hydride in 1 M KOH with 0.1 M NO_3^- . (c) Plots of the current density versus the scan rate for the samples above. (without iR compensation)

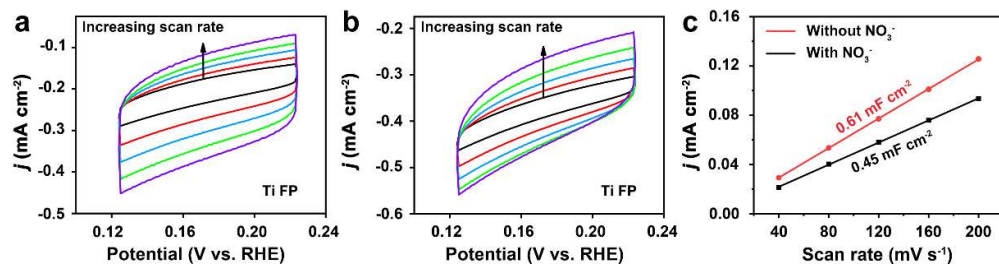


Fig. S23 CV curves of (a) Ti FP in 1 M KOH. (b) Ti FP in 1 M KOH with 0.1 M NO₃⁻.

(c) Plots of the current density versus the scan rate for the samples above. (without iR compensation)

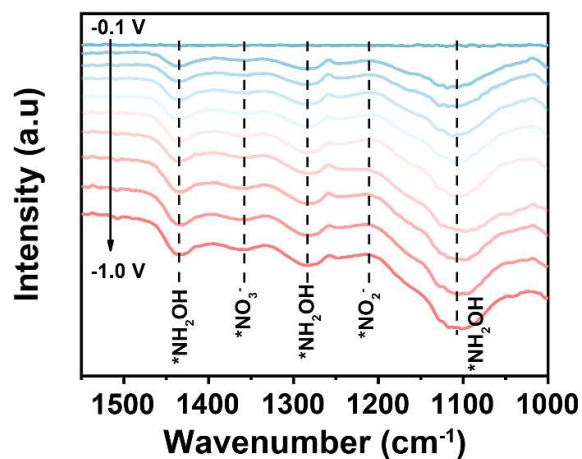


Fig. S24 In-situ ATR FTIR spectra of different intermediates in NIRR pathway.

Note: We employed in-situ Attenuated Total Reflection Fourier Transform Infrared Spectroscopy (ATR-FTIR) to monitor intermediates adsorbed on the titanium hydride. As shown in Fig. S24, five distinct absorption bands were observed in the spectra of $\text{TiH}_{1.97}$ ^{13, 14}. Initially, as the potential increased, the absorption bands at 1354 cm^{-1} , corresponding to the symmetric and asymmetric N-O stretching of NO_3^- , indicated the consumption of NO_3^- . Concurrently, the downward band at 1236 cm^{-1} was attributed to the N-O antisymmetric stretching vibration of NO_2^- , signifying NO_2^- formation from the reduction of NO_3^- . With further negative shift in potential, an intermediate around 1110 cm^{-1} was attributed to the N-O stretching vibration of hydroxylamine (NH_2OH), a crucial intermediate for NH_3 formation. The presence of the characteristic peak of the $-\text{NH}_2$ wagging mode at 1440 cm^{-1} confirmed the formation of NH_3 ¹⁵.

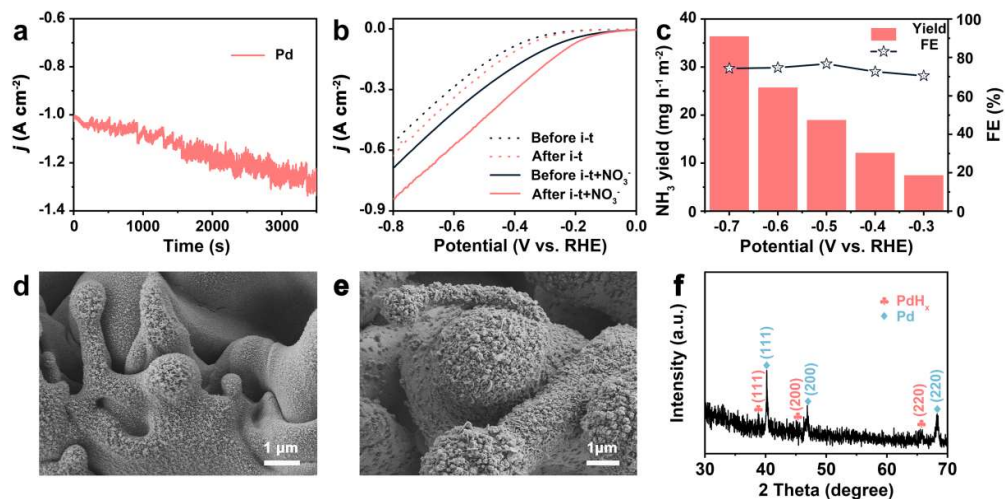


Fig. S25 (a) i-t curves of cathodic electrochemically reconstructed at -1.0 V vs. RHE (without iR compensation). (b) LSV curves (without iR compensation). (c) NH₃ yield and FE for Pd against various work potentials in 1 M KOH solution with 0.1 M NO₃⁻ (without iR compensation). (d, e) SEM images of the Pd before and after cathodic electrochemical reconstruction. (f) XRD patterns.

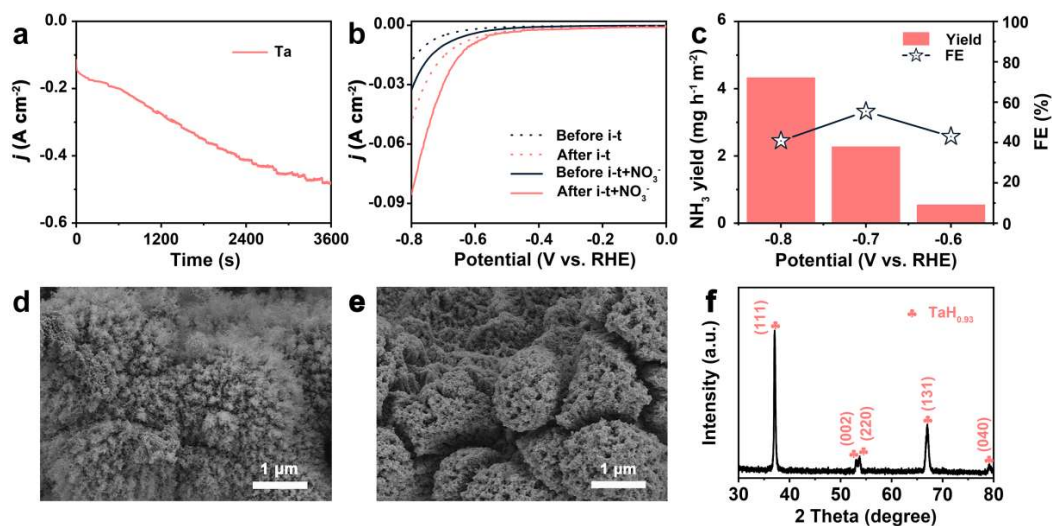


Fig. S26 (a) i-t curves of cathodic electrochemically reconstructed at -0.9 V vs. RHE (without iR compensation). (b) LSV curves (without iR compensation). (c) NH₃ yield and FE for Ta against various work potentials in 1 M KOH solution with 0.1 M NO₃⁻ (without iR compensation). (d, e) SEM images of the Ta before and after cathodic electrochemical reconstruction. (f) XRD patterns.

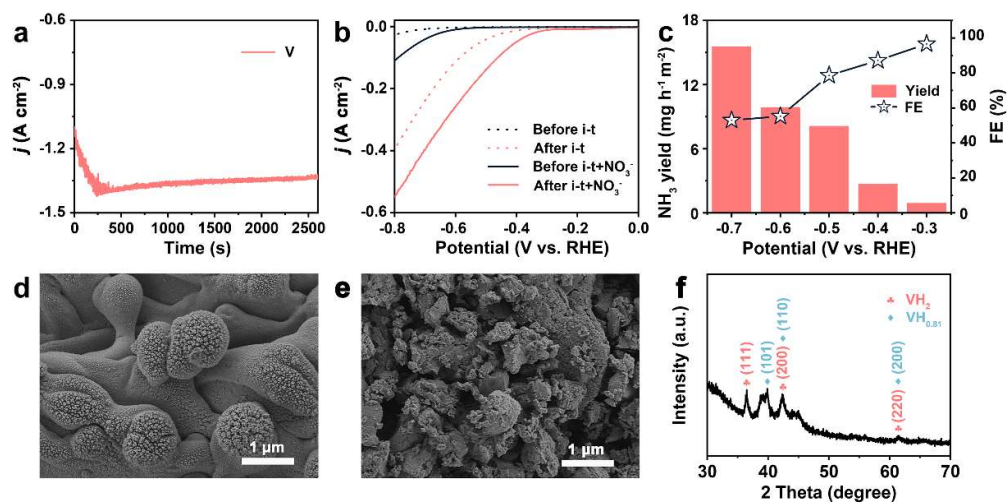


Fig. S27 (a) i-t curves of cathodic electrochemically reconstructed at -1.3 V vs. RHE (without iR compensation). (b) LSV curves (without iR compensation). (c) NH₃ yield and FE for V against various work potentials in 1 M KOH solution with 0.1 M NO₃⁻ (without iR compensation). (d, e) SEM images of the V before and after cathodic electrochemical reconstruction. (f) XRD patterns.

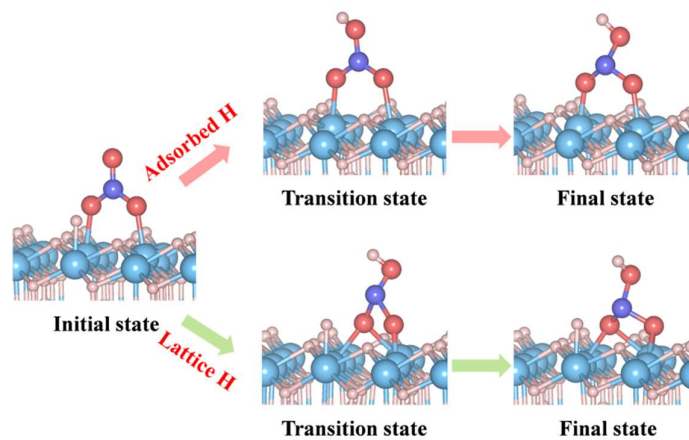


Fig. S28 The configurations of initial state, transition state, and final state for the nitrate hydrogenation through adsorbed H (derived from water splitting) or lattice H (derived from $\text{TiH}_{1.97}$). The light blue, purple, red and pink spheres represent Ti, N, O, and H atoms, respectively.

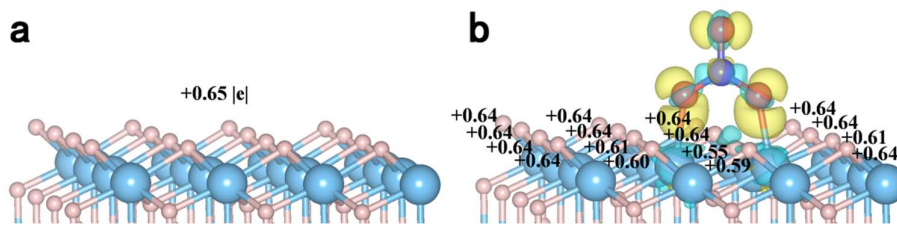


Fig. S29 Calculated Bader charge of surface H **(a)** before and **(b)** after the adsorption of NO_3^- . The yellow section and the blue section represent the charge accumulate and lose region, respectively. The light blue, purple, red and pink spheres represent Ti, N, O, and H atoms, respectively.

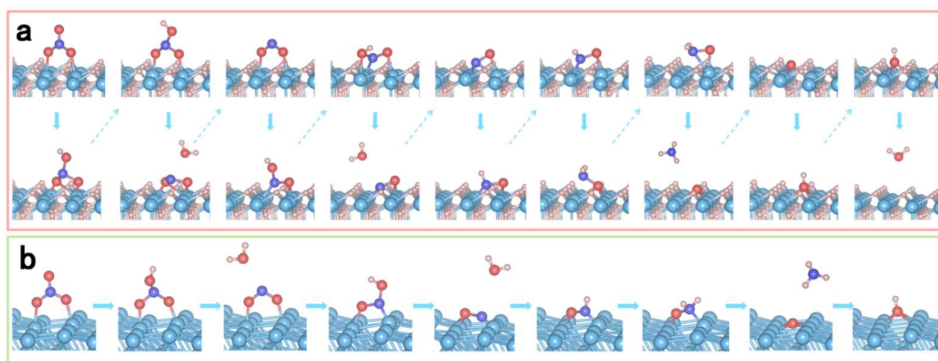


Fig. S30 Adsorption configurations of reaction intermediates during NIRR on **(a)** $\text{TiH}_{1.97}$ and **(b)** Ti. The light blue, purple, red and pink spheres represent Ti, N, O, and H atoms, respectively.

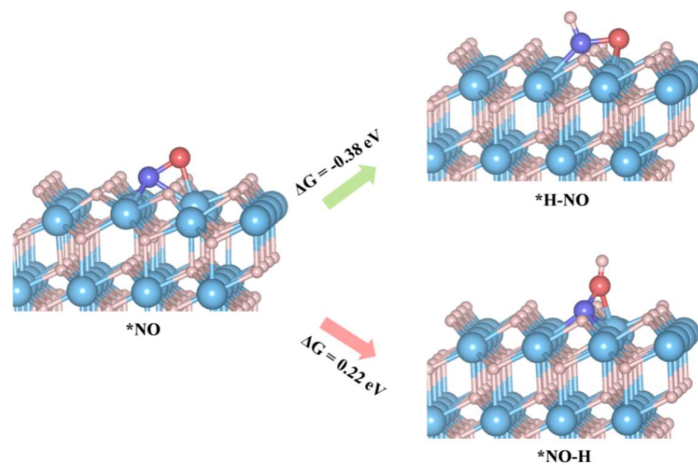


Fig. S31 Calculated reaction free energy from *NO to *NO-H and *H-NO. The light blue, purple, red and pink spheres represent Ti, N, O, and H atoms, respectively.

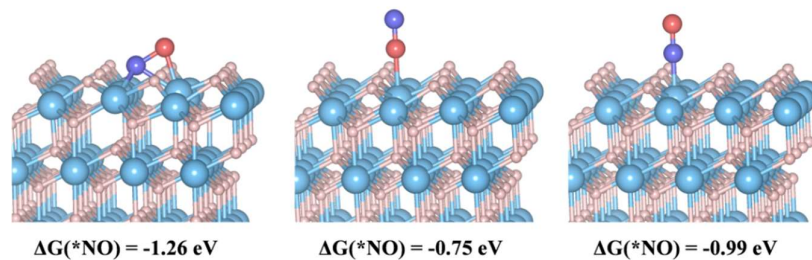


Fig. S32 Different adsorption configurations and corresponding adsorption free energies of NO on $\text{TiH}_{1.97}$. The light blue, purple, red and pink spheres represent Ti, N, O, and H atoms, respectively.

Note: As shown in Fig. S31, it could be found that the reaction free energy from *NO to *NO-H (0.22 eV) was higher than that from *NO to *H-NO (-0.38 eV), indicating the priority of N-terminal of NO during hydrogenation process. In addition, the different adsorption configurations of NO on $\text{TiH}_{1.97}$ were tested, as shown in Fig. S32. By comparing the adsorption free energy of NO, we could conclude that NO tends to adsorb on $\text{TiH}_{1.97}$ in a lying mode with $\Delta G (*NO)$ of -1.26 eV.



Fig. S33 The digital images of H-type electrolytic cell.

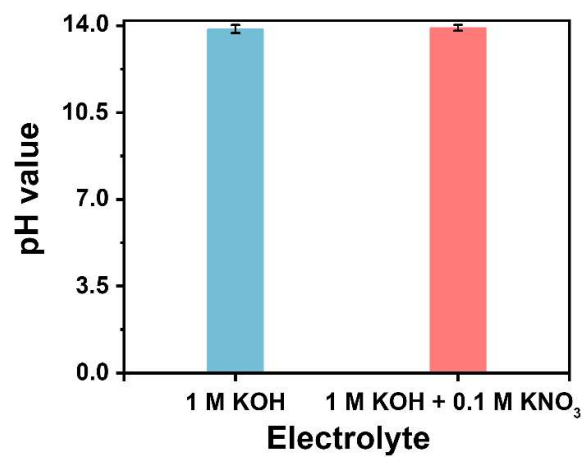


Fig. S34 pH value of the electrolyte. Error bars indicate there lative standard deviations of the mean (n=3).

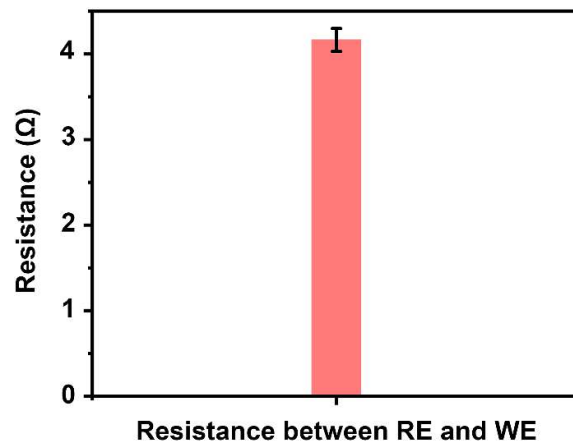


Fig. S35 Resistance of the electrochemical cell in between RE and WE during the constant potential test. Error bars indicate there lative standard deviations of the mean (n=3).

Supplementary Tables

Table S1. Data obtained by fitting Nyquist plots.

Sample	R_s(ohm)	R_p(ohm)	CPE₁(F cm⁻²)	R_{ct}(ohm)	CPE₂(F cm⁻²)
TiH _{1.97} +NO ₃ ⁻	1.55	0.23	0.993	0.82	1.028
TiH _{1.97}	1.803	0.07	1.115	4.751	0.865
Ti+NO ₃ ⁻	1.998	0.252	1.084	1.759	1.047
Ti	2.13	0.174	1.047	19.97	0.823

Table S2. Structural parameters of Ti, TiH_{1.97} and TiH₂ extracted from the EXAFS fitting.

Sample	Scattering path	CN	R(Å)	$\sigma^2/\text{Å}^2$	R factor
TiH _{1.97}	Ti-Ti1.1	12	3.13	0.006	0.011
TiH ₂	Ti-Ti1.1	12	3.14	0.004	0.005
Ti fiol	Ti-Ti1.1	6	2.90	0.012	0.013

The S_0^2 was fixed as 0.7. The interatomic distances (R) and coordination numbers (CN). The CN was the coordination number; R was the half path length of the path, for a single scattering path, it was the inter-atomic distance. σ^2 was the mean square variation in path length, this parameter encapsulates both static and thermal disorder. ΔE_0 was an adjustment to the E_0 used to evaluate the wavenumber of the theory, it is useful to think of ΔE as the parameter which aligns the energy grids of the data and the theory. R factor was used to indicate the accuracy of the fitting. The fitted ranges for k and R spaces were selected to be $k=3-12.4 \text{ Å}^{-1}$ with $R=1.5-3.5 \text{ Å}$ (k^3 -weighted).

Table S3. The comparison of the NH₃ yield and FE with the reported catalysts for NIRR by the area of electrode and ECSA.

Catalyst	FE (%)	Yield _{NH₃} (mg h ⁻¹ cm ⁻²)	ECSA (cm ²)	ECSA-normalized NH ₃ yields	Electrolyte	Reduction Potential (vs. RHE)	Reference
TiH _{1.97}	99.1	83.6	115	0.72	1 M KOH + 0.1 M KNO ₃	-0.70 V	This work
Cu _x S-CO _{0.5}	95.6	2.3	243	0.01	1 M KOH + 0.1 M KNO ₃	-0.40 V	16
o-CoP/C@ Cu ₃ P/CF	90.3	26.7	1603	0.01	1 M KOH + 0.1 M KNO ₃	-0.25 V	17
(Cu _{0.6} Co _{0.4}) Co ₂ O ₄	96.5	18.5	/	/	1 M KOH + 0.1 M NO ₃ ⁻	-0.45 V	18
CuO NWAs @Fe ₃ O ₄	97.5	28.7	147	0.19	1 M KOH + 0.1 M KNO ₃	-0.27 V	19
RuO _x /Pd	98.6	23.5	92	0.24	1 M KOH + 0.1 M KNO ₃	-0.50 V	20
CNs@CoP	98.3	40.4	/	/	1 M KOH + 0.1 M NaNO ₃	-0.60 V	21
Cu ₅₀ Ni ₅₀	90.0	7.1	312	0.02	1 M KOH 0.1 M KNO ₃	-0.15 V	22
FeB ₂	96.8	25.5	123	0.20	1 M KOH + 0.1 M KNO ₃	-0.60 V	23
Cu@C	99.3	25.3	587	0.04	1 M KOH + 0.1 M KNO ₃	-0.70 V	24
CuFe-450	95.1	14.1	/	/	1 M KOH + 0.1 M KNO ₃	-0.30 V	25

Table S4. The comparison of the NH₃ yield and FE with the reported catalysts for NIRr by the weight of catalyst.

Catalyst	FE (%)	Yield _{NH₃} (mg h ⁻¹ mg _{cat} ⁻¹)	Electrolyte	Reduction Potential (vs. RHE)	Reference
TiH _{1.97}	99.1	139.3	1 M KOH + 0.1 M KNO ₃	-0.70 V	This work
AuCu ₃ @Au	86.5	134.3	1 M KOH + 0.5 M NO ₃ ⁻	-0.75 V	26
Bi-Cl _{red}	73.5	10.0	1 M KOH + 0.1 M NO ₃ ⁻	-0.70 V	27
Cu/Cu _x O/GDY	96.1	18.7	1 M KOH + 0.1 M NO ₃ ⁻	-0.70 V	28
Cu ₃ N/GDY	84.5	18.4	1 M KOH + 0.1 M KNO ₃	-0.70 V	29
2D Fe-cyano	82.3	53.5	1 M KOH 0.1 M KNO ₃	-0.60 V	30

Geometrical coordinates of model structures

The fractional coordinates of all the models in this manuscript are listed below (The cell parameters are shown at the beginning of the coordinates of each model, and are given in the unit of angstrom).

Ti(101)

10.4314664725790429	-2.8498194856268833	-0.0768779622810153
-0.0166803521858506	11.3379161377095912	0.0017974789564654
-0.1698463532651056	0.0037600665585584	26.7200057729027627

Ti

64

Selective dynamics

Direct

0.0659899999999993	0.0154339999999991	0.0657059999999987
0.1753882744338817	0.1678265344161589	0.1444294786868257
0.2972108884537795	0.0728435973188790	0.2295640445332805
0.4081624675553481	0.2256674186357692	0.3095293356456589
0.2968440000000001	0.1981469999999987	0.0508159999999975
0.4060960506130432	0.1009556161847060	0.1323097295622069
0.0291032698322626	0.0065376661865054	0.2177864304091265
0.1386650350906152	0.1590399585264097	0.2976103142667195
0.5659899999999993	0.0154339999999991	0.0657059999999987
0.6753645430721228	0.1678195353065752	0.1444344836291264

0.7972004195417257 0.0728413489072687 0.2295825188882551
0.9081959480523664 0.2256781227634999 0.3095297198778511
0.7968440000000001 0.1981469999999987 0.0508159999999975
0.9061142724551446 0.1009592082140587 0.1323241292090252
0.5290727853781260 0.0065301717686472 0.2177753335319663
0.6386217190920472 0.1590261072242957 0.2976107899013476
0.0659899999999993 0.2654339999999991 0.0657059999999987
0.1753874217871217 0.4178269534267967 0.1444294959465834
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0.4081696380643718 0.4756662815969637 0.3095280840680039
0.2968440000000001 0.4481469999999987 0.0508159999999975
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0.5659899999999993 0.2654339999999991 0.0657059999999987
0.6753634481997719 0.4178186558522883 0.1444341413615123
0.7972027366323258 0.3228407838930245 0.2295830309504623
0.9082001968391301 0.4756792211617145 0.3095302249989040
0.7968440000000001 0.4481469999999987 0.0508159999999975
0.9061126945777317 0.3509590167266472 0.1323220241337688
0.5290753871532758 0.2565299807675750 0.2177779765692665
0.6386187053877572 0.4090237521754186 0.2976103537273901

0.065989999999993 0.515433999999991 0.0657059999999987
0.1753933875732685 0.6678293432144145 0.1444279672656130
0.2972083604839114 0.5728405404697380 0.2295659107859490
0.4081684683092975 0.7256642294982686 0.3095318725749728
0.296844000000001 0.6981469999999987 0.0508159999999975
0.4060954210757104 0.6009522048219141 0.1323091584969938
0.0291018002594874 0.5065369109110717 0.2177887279896432
0.1386640035791839 0.6590379279109878 0.2976150479631096
0.565989999999993 0.515433999999991 0.0657059999999987
0.6753668464932472 0.6678220167940258 0.1444335367741927
0.7971953495749551 0.5728353937896790 0.2295823706990058
0.9081965384002830 0.7256734961902320 0.3095331936144327
0.796844000000001 0.6981469999999987 0.0508159999999975
0.9061140183423044 0.6009561262957062 0.1323231791651972
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0.065989999999993 0.765433999999991 0.0657059999999987
0.1753944917022584 0.9178298106179643 0.1444280330899840
0.2972044706314446 0.8228389085736708 0.2295648094641252
0.4081634757189476 0.9756630874042416 0.3095312074911820
0.296844000000001 0.9481469999999987 0.0508159999999975
0.4060989557539990 0.8509535186577960 0.1323109190373978

0.0291012949491383	0.7565354345754238	0.2177875629587963
0.1386641241755602	0.9090401593503729	0.2976134053267718
0.5659899999999993	0.7654339999999991	0.0657059999999987
0.6753667454850237	0.9178190947485994	0.1444328346352961
0.7971926087395153	0.8228347836170710	0.2295815671230298
0.9081920410486743	0.9756744878254594	0.3095325390910299
0.7968440000000001	0.9481469999999987	0.0508159999999975
0.9061151476814179	0.8509564420374890	0.1323252386872790
0.5290712373735174	0.7565287889622669	0.2177764917676430
0.6386207749769335	0.9090275700033296	0.2976132642914052

TiH_{1.97}(111)

10.1930449999999997	-5.9205470000000000	0.0221310000000000
0.0000000000000000	11.7965789999999995	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H Ti

96 48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.5705460000000002	0.3465610000000012	0.0195900000000009

0.5705460000000002	0.8465610000000012	0.0195900000000009
0.4037973730641831	0.0132679332543363	0.1240625484983642
0.4037973662868792	0.5132679331579505	0.1240625517712606
0.9037973712717723	0.0132679333530412	0.1240625524068027
0.9037973821489759	0.5132679346967804	0.1240625471825813
0.2371271793657306	0.1799691484121072	0.2250741615878554
0.2371271783927762	0.6799691491862792	0.2250741623697517
0.7371271748569733	0.1799691455555109	0.2250741618485901
0.7371271833170469	0.6799691489821034	0.2250741610776703
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.9867330000000010	0.4300550000000030	0.0814719999999980
0.9867330000000010	0.9300550000000030	0.0814719999999980
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0.3200765100683871	0.5967381506070932	0.1824955155057124
0.8200765117596915	0.0967381504943532	0.1824955148789288
0.8200765152920347	0.5967381599058882	0.1824955177489752
0.1533241358977681	0.2634581185399287	0.2869429519262829
0.1533241344967762	0.7634581202415357	0.2869429508678379
0.6533241323370576	0.2634581163110845	0.2869429511415093
0.6533241371957478	0.7634581221127108	0.2869429522670304
0.0705460000000002	0.0965610000000012	0.0195900000000009

0.0705460000000002	0.5965610000000012	0.0195900000000009
0.5705460000000002	0.0965610000000012	0.0195900000000009
0.5705460000000002	0.5965610000000012	0.0195900000000009
0.4037973730069088	0.2632679402566502	0.1240625515512706
0.4037973771015553	0.7632679415984529	0.1240625513643570
0.9037973812497945	0.2632679468096161	0.1240625513322623
0.9037973817637485	0.7632679480748099	0.1240625522960703
0.2371271667086438	0.4299691314880146	0.2250741619774803
0.2371271621056261	0.9299691279555931	0.2250741637006383
0.7371271637354009	0.4299691306410211	0.2250741639875584
0.7371271677614509	0.9299691333168203	0.2250741608172170
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0.9867330000000010	0.1800550000000030	0.0814719999999980
0.9867330000000010	0.6800550000000030	0.0814719999999980
0.3200765106929122	0.3467381620587471	0.1824955180237874
0.3200765155040332	0.8467381619842447	0.1824955191519916
0.8200765246405270	0.3467381640510864	0.1824955182780433
0.8200765188591365	0.8467381696091213	0.1824955169270850
0.1533241252303786	0.0134580917176403	0.2869429516649895
0.1533241275384368	0.5134580977285848	0.2869429520773121
0.6533241277722287	0.0134580998607679	0.2869429517581253

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0.3205450000000027	0.5965610000000012	0.0195900000000009
0.8205450000000027	0.0965610000000012	0.0195900000000009
0.8205450000000027	0.5965610000000012	0.0195900000000009
0.1537973667622064	0.2632679395897629	0.1240625519840692
0.1537973660267594	0.7632679354274751	0.1240625494681939
0.6537973612681443	0.2632679297183489	0.1240625504965761
0.6537973633504961	0.7632679419595664	0.1240625536582469
0.4871271730225562	0.4299691242548633	0.2250741611917909
0.4871271735511871	0.9299691351582149	0.2250741614969958
0.9871271772374396	0.4299691347049595	0.2250741599522312
0.9871271802672230	0.9299691310503759	0.2250741605948621
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0.2367330000000010	0.6800550000000030	0.0814719999999980
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0.7367330000000010	0.6800550000000030	0.0814719999999980
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0.0700765013756204	0.8467381588068664	0.1824955209927803
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0.4033241276442404	0.5134581006968776	0.2869429526277278
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0.8205450000000027	0.3465610000000012	0.0195900000000009
0.8205450000000027	0.8465599999999966	0.0195900000000009
0.1537973577188794	0.0132679292995357	0.1240625471947831
0.1537973588414595	0.5132679242262208	0.1240625493247605
0.6537973614069162	0.0132679243802763	0.1240625485109559
0.6537973567734786	0.5132679287519974	0.1240625463722657
0.4871271850969848	0.1799691546205131	0.2250741622268690
0.4871271777264267	0.6799691538113720	0.2250741593064227
0.9871271829964607	0.1799691546978415	0.2250741604956313
0.9871271865453765	0.6799691578089684	0.2250741625193874
0.2367330000000010	0.4300550000000030	0.0814719999999980
0.2367330000000010	0.9300550000000030	0.0814719999999980
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.7367330000000010	0.9300550000000030	0.0814719999999980
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0.0700764972424342	0.5967381433707597	0.1824955156084360
0.5700764987436814	0.0967381477435481	0.1824955168025285

0.5700764962640080	0.5967381488818855	0.1824955142625755
0.4033241470415045	0.2634581223171322	0.2869429510789804
0.4033241428055427	0.7634581185392760	0.2869429508373848
0.9033241454595291	0.2634581186788887	0.2869429517386012
0.9033241500001237	0.7634581216042498	0.2869429517765429
0.403638999999983	0.2633080000000021	0.0542870000000022
0.403638999999983	0.7633080000000021	0.0542870000000022
0.903638999999983	0.2633080000000021	0.0542870000000022
0.903638999999983	0.7633080000000021	0.0542870000000022
0.2369387155614366	0.4300029937437586	0.1532774145735026
0.2369387874250068	0.9300029618825217	0.1532774070556027
0.7369388971343347	0.4300030087550806	0.1532774047967755
0.7369388508884887	0.9300030916921670	0.1532774151218799
0.0702279412553343	0.0967160521191031	0.2522567141789921
0.0702279324302170	0.5967160371830332	0.2522567491272981
0.5702279334513940	0.0967160414931771	0.2522567463341462
0.5702279200985864	0.5967160350703207	0.2522567312670181
0.403638999999983	0.0133080000000021	0.0542870000000022
0.403638999999983	0.5133080000000021	0.0542870000000022
0.903638999999983	0.0133080000000021	0.0542870000000022
0.903638999999983	0.5133080000000021	0.0542870000000022
0.2369387809491137	0.1800029983814461	0.1532774167052289

0.2369387293644310	0.6800029658183383	0.1532774080590995
0.7369388742314898	0.1800030554010293	0.1532774075101773
0.7369388941762661	0.6800030381331866	0.1532774070587276
0.0702279258256140	0.3467160572556076	0.2522567324606705
0.0702279503988458	0.8467160308722830	0.2522567196197305
0.5702279335517206	0.3467160189480015	0.2522567339783961
0.5702279207280065	0.8467160709430498	0.2522567360460351
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.4869388204384464	0.1800029762987099	0.1532774108540299
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0.9869388355094549	0.1800030920646287	0.1532774093451676
0.9869388657150185	0.6800029877732585	0.1532774107779568
0.3202279223008422	0.3467160391014216	0.2522567286805544
0.3202279262975067	0.8467160358994235	0.2522567398945007
0.8202279534784397	0.3467160501775234	0.2522567396614581
0.8202279557335328	0.8467160662166029	0.2522567230672317
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.6536389999999983	0.2633080000000021	0.0542870000000022

0.653638999999983	0.763308000000021	0.054287000000022
0.4869387749206365	0.4300029536330112	0.1532774125073662
0.4869388013591360	0.9300030293479690	0.1532774078046721
0.9869388581507802	0.4300030388012578	0.1532774067453610
0.9869388590525533	0.9300030257115144	0.1532774107754805
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0.3202279053144166	0.5967160410966115	0.2522567441936456
0.8202279323307091	0.0967160623379376	0.2522567359099399
0.8202279691440931	0.5967160390886004	0.2522567371834609

Ti(101)-H

10.3841267536841411	-2.8576068351851118	-0.1464140441106770
-0.0005686340597545	11.3067771504924810	0.0030753216658324
-0.0029841504721516	-0.0008952147430414	26.9040727632061518

H Ti

1 64

Selective dynamics

Direct

0.5777251496599519	0.5188093257664327	0.3441776037113592
0.0659899999999993	0.0154339999999991	0.0657059999999987
0.1750200472899324	0.1677481063171287	0.1440675582937431
0.2967810845122383	0.0728022216015600	0.2287165605780378

0.4075402284008403 0.2250213286479562 0.3073460376296416
0.2968440000000001 0.1981469999999987 0.0508159999999975
0.4060150865414087 0.1007561476948328 0.1316766281091224
0.0286073468342777 0.0064045874915921 0.2169936331632047
0.1375802429649469 0.1590297166410465 0.2964378726844926
0.5659899999999993 0.0154339999999991 0.0657059999999987
0.6750665669746237 0.1673912598961938 0.1441946736369973
0.7963715327101619 0.0727079459573128 0.2288187800255974
0.9067046442391059 0.2255559649153914 0.3084950553209737
0.7968440000000001 0.1981469999999987 0.0508159999999975
0.9055900833430873 0.1009340548779932 0.1318449697483116
0.5280159248409312 0.0060465946260651 0.217310098877278
0.6383113855416936 0.1587694143530024 0.2962741103405243
0.0659899999999993 0.2654339999999991 0.0657059999999987
0.1748275862041107 0.4177800588227527 0.1440742525704961
0.2962488239316677 0.3226237831349483 0.2290129821065297
0.4091060758749053 0.4764384814233529 0.3103600462085043
0.2968440000000001 0.4481469999999987 0.0508159999999975
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0.0283955881804230 0.2565822589316472 0.2169353492985557
0.1357761266714347 0.4086406470303525 0.2965022756245613
0.5659899999999993 0.2654339999999991 0.0657059999999987

0.6753209595276458 0.4179645231286698 0.1437086527589150
0.7971895025817263 0.3227664043040462 0.2286514176553675
0.9054246810509993 0.4750541024601335 0.3078022838948438
0.7968440000000001 0.4481469999999987 0.0508159999999975
0.9064821978985209 0.3509013311951568 0.1317214218015343
0.5292850017492126 0.2575104896251407 0.2161844656627212
0.6348077056059084 0.4109974903807357 0.2978248800094244
0.0659899999999993 0.5154339999999991 0.0657059999999987
0.1745251557646639 0.6678469216307544 0.1441168656049392
0.2954694985252136 0.5729165773748411 0.2289985821365324
0.4076449817930446 0.7262992805718982 0.3073055192511581
0.2968440000000001 0.6981469999999987 0.0508159999999975
0.4056800842402406 0.6007271188483138 0.1316881711742762
0.0273908854669019 0.5066932118555101 0.2168499164464870
0.1378865057248128 0.6588325276706322 0.2966922464678072
0.5659899999999993 0.5154339999999991 0.0657059999999987
0.6750163685667641 0.6676543495703759 0.1436511968785751
0.7930428081974412 0.5718399144800755 0.2287024418034204
0.9055791960326240 0.7249062092925648 0.3079328365306906
0.7968440000000001 0.6981469999999987 0.0508159999999975
0.9061553614386092 0.6011053380247051 0.1318367861492556
0.5265042942113290 0.5061926744552655 0.2168566527532763

0.6352366787710189	0.6554277009355726	0.2979135761978146
0.0659899999999993	0.7654339999999991	0.0657059999999987
0.1750332697483218	0.9177396594062289	0.1441453944493826
0.2961217736264506	0.8226128173447347	0.2287711662375790
0.4069789987188769	0.9751624596188460	0.3089385069071289
0.2968440000000001	0.9481469999999987	0.0508159999999975
0.4060476370490612	0.8511538401868152	0.1317426718239839
0.0277164037639121	0.7556106152541023	0.2170387246702393
0.1365733869305838	0.9085146600899918	0.2964399296171636
0.5659899999999993	0.7654339999999991	0.0657059999999987
0.6749389489426046	0.9180814339547474	0.1441164310363668
0.7974814778818413	0.8230371695868887	0.2285752441021869
0.9067521758424865	0.9750583864959702	0.3085923747049011
0.7968440000000001	0.9481469999999987	0.0508159999999975
0.9063238912118268	0.8512839273867400	0.1316124946576703
0.5293809761095160	0.7556649346889412	0.2162630651825941
0.6385949137940502	0.9093383059757015	0.2963568953533730

TiH_{1.97}(111)-H

10.1930359999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H Ti

97 48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4037641193345765	0.0132635739467114	0.1239308376548757
0.2363397384000438	0.1788198143916681	0.2244046671594599
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3199658565063230	0.0965874024629623	0.1820000969018314
0.1529547622469571	0.2635239791770166	0.2860054832548229
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4038399724901435	0.2634445057086453	0.1241326881458476
0.2358122655069878	0.4294925813909268	0.2243273648591003
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3198524795267623	0.3466962297430148	0.1819067583661299
0.1532389630215674	0.0134017147822065	0.2863679200578870
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1537027816128883	0.2632011457768748	0.1239234829758059
0.4878896736341713	0.4320655555759951	0.2255986782564563
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0697541561286360	0.3466258677902796	0.1819522026200235
0.4032088176334055	0.0134139829955199	0.2863912804769786

0.3205450000000027	0.3465599999999966	0.0195900000000009
0.1537594639069073	0.0132519862485383	0.1239370098387857
0.4864533367568938	0.1789560858370872	0.2244220411923077
0.2367330000000010	0.4300550000000030	0.0814719999999980
0.0700664295701163	0.0966919387008905	0.1820414072641351
0.4027162014295205	0.2625509360271666	0.2855264739257357
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.9038069783087322	0.0133044271228008	0.1239241186476213
0.7367364132439463	0.1800031734396107	0.2245127497823483
0.9867330000000010	0.4300550000000030	0.0814719999999980
0.8201324262788617	0.0969899330177749	0.1819624036807262
0.6533216212832397	0.2634714009616267	0.2860173513667708
0.5705460000000002	0.0965599999999966	0.0195900000000009
0.9037688697030629	0.2632546332531276	0.1239756308161501
0.7374178687915965	0.4295338140490807	0.2243477575144537
0.9867330000000010	0.1800550000000030	0.0814719999999980
0.8200931583800545	0.3466806555994966	0.1819657925333298
0.6533867126010713	0.0136366582851651	0.2860354238842948
0.8205460000000002	0.0965599999999966	0.0195900000000009
0.6537834602675842	0.2632783959873824	0.1239440306875138
0.9869430853521131	0.4302327952256095	0.2245046089116600
0.7367330000000010	0.1800539999999984	0.0814719999999980

0.5700530038113347	0.3467534515441246	0.1819046814273513
0.9030948834417805	0.0136531393390891	0.2860189100059240
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6537698693840013	0.0132748328571910	0.1239376357840899
0.9870053424647930	0.1799053039756184	0.2245511833548806
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5699580509945493	0.0967529177039755	0.1820151130088699
0.9031626941386249	0.2634618395248079	0.2863550335821341
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4036481923049691	0.5132291839745882	0.1241128962262543
0.2362915622845368	0.6806022344802611	0.2243534409340349
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3198356997955226	0.5966562049288451	0.1818639074282245
0.1532405878524621	0.7634698944325308	0.2863852123036181
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4038632784948646	0.7631806012365990	0.1241464968334264
0.2369908662228533	0.9299624560464752	0.2244665628749867
0.4867330000000010	0.6800539999999984	0.0814719999999980
0.3199475769961749	0.8468541576663037	0.1819997522932457
0.1529819723136744	0.5132674185732907	0.2860136124320330
0.3205450000000027	0.5965610000000012	0.0195900000000009
0.1537781738189183	0.7633033430122337	0.1239254567217852

0.4863978966813159 0.9306167171977472 0.2243767538375448
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0702069988162935 0.8468363486116269 0.1819957905759220
0.3962838747836085 0.5101046892733954 0.2850246928010063
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1537456658394744 0.5132723031222066 0.1239346133234867
0.4879362996097797 0.6789813511126248 0.2256238862367563
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0700207578299653 0.5968354093350120 0.1820032986391916
0.4027434502187782 0.7638571155858883 0.2855949602414596
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9037521343531195 0.5132622411789060 0.1239427319558937
0.7347914501554430 0.6789958349819585 0.2255997630811974
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8200371866954361 0.5967341402153337 0.1818957739127397
0.6565176560248607 0.7701987356585585 0.2851398263902268
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9035691871374365 0.7631891648534299 0.1241301745785413
0.7374301209280376 0.9310816701242067 0.2243489882356229
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8200546949908388 0.8468925652838487 0.1819254035385457
0.6566177713092654 0.5101195247581173 0.2851360867906066

0.8205460000000002	0.5965610000000012	0.0195900000000009
0.6537942497025273	0.7633675397912191	0.1241121782883050
0.9880573920759426	0.9305573139568397	0.2244120725003672
0.7367330000000010	0.6800550000000030	0.0814719999999980
0.5701277982946668	0.8469095805954552	0.1818936125141015
0.9031841694318863	0.5133468336829472	0.2860143367415735
0.8205460000000002	0.8465610000000012	0.0195900000000009
0.6537500150867940	0.5132787059947072	0.1241443523360650
0.9879993264857919	0.6805260553636423	0.2244067114084480
0.7367330000000010	0.9300550000000030	0.0814719999999980
0.5699789760548508	0.5967599041279817	0.1809506429467929
0.9040687063191037	0.7638939309891302	0.2855370874063303
0.5689950705063868	0.5961398706496990	0.3212054074537178
0.4036389999999983	0.2633080000000021	0.0542870000000022
0.2367101243591893	0.4298550041841615	0.1530176653840883
0.0700836415153843	0.0966591121604712	0.2517927495367424
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.2367932548173538	0.1798652449668144	0.1529618163354045
0.0691586238411406	0.3463837238104233	0.2515676889913308
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4868493399034267	0.1799165845950595	0.1529410578090656
0.3191096646499677	0.3456710431659681	0.2512946222997298

0.153638999999983 0.263308000000021 0.054287000000022
0.4871088410090030 0.4305924959786420 0.1534029588368621
0.3199105755028150 0.0964054606838538 0.2516220762424347
0.903638999999983 0.263308000000021 0.054287000000022
0.7368899933036702 0.4300123326674815 0.1530509231358083
0.5699278784655192 0.0966539778495722 0.2517591155868181
0.903638999999983 0.013308000000021 0.054287000000022
0.7368109889912462 0.1799975599311692 0.1529567175476821
0.5698118360291228 0.3457714869904968 0.2513110402193620
0.653638999999983 0.013308000000021 0.054287000000022
0.9869410521343147 0.1799344774169863 0.1529777657517110
0.8203933555849053 0.3464154926316527 0.2516147462580015
0.653638999999983 0.263308000000021 0.054287000000022
0.9868944934118387 0.4300947478152495 0.1529522802961255
0.8203926999762883 0.0975865285592485 0.2515766288383317
0.403638999999983 0.763308000000021 0.054287000000022
0.2368904807486683 0.9300425265925596 0.1530004631141915
0.0701181496381806 0.5968887385914867 0.2517512097543584
0.403638999999983 0.513308000000021 0.054287000000022
0.2367993181328837 0.6800662955439509 0.1529555652098598
0.0703910449366476 0.8468901823423463 0.2516183126969811
0.153638999999983 0.513308000000021 0.054287000000022

0.4871784851786039	0.6797197541300948	0.1534128899553756
0.3199789882940288	0.8468268686556585	0.2516620446492437
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.4868646155261721	0.9301021682024017	0.1529660412399685
0.3190598906474781	0.5970421458149270	0.2512693051581915
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7370311148457972	0.9301595106859860	0.1530283808697182
0.5700118464994235	0.5966654816854471	0.2576570623343303
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7363071227882712	0.6797907198912758	0.1533977815528337
0.5697515615549990	0.8476602510962827	0.2513083091784813
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9869960380639772	0.6800821057172782	0.1529345869386967
0.8210602536205029	0.8476031720461153	0.2513181634499588
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9870193608676922	0.9301005726593682	0.1529655638386557
0.8210393556300992	0.5970031778177458	0.2513016825930370

TiH_{1.97}(111)-H-vacancy

10.1930449999999997	-5.9205470000000000	0.0221310000000000
0.0000000000000000	11.7965789999999995	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H Ti

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Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.5705460000000002	0.8465610000000012	0.0195900000000009
0.4039409463441657	0.0133478751337591	0.1239805941324322
0.4037679142746602	0.5132872284301132	0.1240742114778097
0.9036934438684707	0.0133603549007856	0.1239777744207472
0.9037059364333346	0.5131117555456611	0.1239806775501883
0.2360303719621353	0.1781976233413999	0.2240639130098112
0.2359300398364512	0.6810865727101288	0.2240529275380295
0.7369637622616874	0.1800528642776430	0.2246546034767730
0.7387485998218881	0.6809510302461889	0.2240710125714259
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.9867330000000010	0.4300550000000030	0.0814719999999980
0.9867330000000010	0.9300550000000030	0.0814719999999980
0.3200592748675581	0.0965609699802765	0.1820973505837039
0.3196468832213117	0.5971533509741669	0.1820121752455357

0.8199906018493035	0.0968082758645288	0.1822117381158504
0.8202301826893910	0.5967400476784288	0.1820992617689921
0.1528189260011979	0.2624909336628092	0.2867672312643390
0.1529946932929649	0.7637039548883163	0.2863700474537274
0.6528555154207956	0.2638557151155234	0.2861901890755205
0.6541762865659879	0.7638747741430584	0.2867658684721864
0.0705460000000002	0.0965610000000012	0.0195900000000009
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.5705460000000002	0.0965610000000012	0.0195900000000009
0.5705460000000002	0.5965610000000012	0.0195900000000009
0.4038589285647420	0.2633005555142314	0.1239891012800867
0.4038688439132965	0.7633605463328783	0.1239859320172793
0.9037888157346594	0.2632968461941187	0.1239971365079769
0.9041732128990705	0.7634683672807033	0.1238937386209369
0.2391393848238038	0.4311487970034366	0.2252763866284478
0.2367405888997537	0.9299592006427371	0.2244770067230570
0.7365380551579520	0.4298379351209347	0.2247827668629243
0.7365024752186807	0.9297722346677721	0.2248070860549589
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.4867330000000010	0.6800550000000030	0.0814719999999980
0.9867330000000010	0.1800550000000030	0.0814719999999980
0.9867330000000010	0.6800550000000030	0.0814719999999980

0.3196593624346284 0.3460316103764086 0.1820404929588431
0.3200628644217497 0.8469957183412571 0.1821190072343338
0.8199900772458005 0.3467040763728836 0.1822152100083560
0.8201988473416755 0.8469785340080854 0.1821047450288002
0.1530831690804312 0.0132201635666206 0.2863497246746123
0.1528437853085469 0.5142129307780536 0.2867563960710947
0.6528324976766803 0.0127609799460494 0.2861631684798861
0.6542006204327812 0.5140786188303567 0.2867543610975664
0.3205450000000027 0.0965610000000012 0.0195900000000009
0.3205450000000027 0.5965610000000012 0.0195900000000009
0.8205450000000027 0.0965610000000012 0.0195900000000009
0.8205450000000027 0.5965610000000012 0.0195900000000009
0.1536945170510875 0.2632803646444503 0.1239951284082458
0.1535929675919742 0.7634583462378264 0.1238845249777972
0.6537582849360891 0.2632962070822003 0.1240008586518505
0.6537717803377890 0.7633574281653396 0.1239951358979167
0.4859496952768043 0.4310265478596088 0.2252399495481886
0.4871050186475536 0.9297978576008920 0.2248073244612633
0.9872223642439345 0.4298974766470935 0.2248093793941636
0.9870423087664861 0.9299412765738868 0.2244765721406680
0.2367330000000010 0.1800550000000030 0.0814719999999980
0.2367330000000010 0.6800550000000030 0.0814719999999980

0.736733000000010	0.180055000000030	0.081471999999980
0.736733000000010	0.680055000000030	0.081471999999980
0.0703438001081223	0.3469187415697618	0.1822934476306569
0.0700314905522364	0.8467634615166160	0.1820452320714537
0.5698809098521110	0.3469221359496148	0.1822821366712695
0.5698821304481168	0.8464603908508417	0.1822920435068529
0.4034265961840682	0.0136836617493396	0.2865628454936989
0.9030801534399787	0.0136120058846651	0.2865286356511658
0.9030215837948099	0.5132870357324850	0.2865584407027610
0.3205450000000027	0.3465610000000012	0.0195900000000009
0.3205450000000027	0.8465599999999966	0.0195900000000009
0.8205450000000027	0.3465610000000012	0.0195900000000009
0.8205450000000027	0.8465599999999966	0.0195900000000009
0.1535821715315614	0.0128810008920583	0.1238935638913328
0.1536944176332619	0.5131868932249163	0.1239865938281251
0.6537573223226697	0.0132652673299982	0.1239969525502968
0.6537553300105480	0.5131993060132704	0.1239898081381333
0.4871705059359271	0.1804619146945780	0.2247815852520893
0.4858691665658560	0.6779078279078331	0.2252687606655076
0.9872384372625324	0.1805028875287230	0.2248063505854172
0.9870328890417980	0.6802539700047574	0.2244804741176996
0.2367330000000010	0.4300550000000030	0.081471999999980

0.236733000000010	0.930055000000030	0.081471999999980
0.736733000000010	0.430055000000030	0.081471999999980
0.736733000000010	0.930055000000030	0.081471999999980
0.0698174968339761	0.0965956215034640	0.1821020188528534
0.0698090298633269	0.5967361633289968	0.1821184389966360
0.5700962975945721	0.0968099354441257	0.1822154577685103
0.5707575731406686	0.5971354007660814	0.1820487250284523
0.4026054067600091	0.2624680710876957	0.2867495537760413
0.4024907818826433	0.7638682576085307	0.2867526150300810
0.9039601408005561	0.2638803408853406	0.2861587000070723
0.9034705161777737	0.7636114006192644	0.2863512451995872
0.403638999999983	0.263308000000021	0.054287000000022
0.403638999999983	0.763308000000021	0.054287000000022
0.903638999999983	0.263308000000021	0.054287000000022
0.903638999999983	0.763308000000021	0.054287000000022
0.2367998896671855	0.4299556786124379	0.1531841216683353
0.2369769410352834	0.9300291301217858	0.1529848187342325
0.7368833767196125	0.4299582512420888	0.1531130457451978
0.7368796207183211	0.9300943869373832	0.1531076565052052
0.0696867076884428	0.0962320300576818	0.2518287720346601
0.0696798397367117	0.5970026564203170	0.2518445243663416
0.5700840919219559	0.0968217200532521	0.2518258265365418

0.5732640716906606	0.5983322961888760	0.2515689081206943
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.2367078838842746	0.1795937278067214	0.1528699525256597
0.2366718475242680	0.6802506112651897	0.1528675097761429
0.7369037324760003	0.1800212724544335	0.1530908743200668
0.7373269625783715	0.6802178480288792	0.1528760368261228
0.0714797762307220	0.3475632830345934	0.2519918322930717
0.0700489200046913	0.8467963800664499	0.2517189947661037
0.5694122721622740	0.3474271338695556	0.2519756563850875
0.5693020089841068	0.8454018531135944	0.2519899002831893
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.4869687746654314	0.1800438924084580	0.1531125429811097
0.4869777933827494	0.6801299666718414	0.1531837545154714
0.9868347442376687	0.1800446332602519	0.1531075236457063
0.9868962828318498	0.6799522205251457	0.1529867728004452
0.3184833546147417	0.3435098675635758	0.2515581220475069

0.3198430903937302	0.8471779482188569	0.2518462525618972
0.8200367497925329	0.3467723861941334	0.2518247327106394
0.8205935869860899	0.8471424622429740	0.2518309548873806
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.4869482274965357	0.4299875168138312	0.1531850978924699
0.4870105132881059	0.9300911925622293	0.1531243374504824
0.9868396512813359	0.4299194103900654	0.1531249142082179
0.9868630518455057	0.9300660970241829	0.1530006062525567
0.3199101771381398	0.0962803277243858	0.2518105851270409
0.3183219868235795	0.5985429837551568	0.2514786320407560
0.8200500798710584	0.0967996420032150	0.2517994460208255
0.8205418914663341	0.5969370594379486	0.2518105288796687

Ti(101)-NO₃

10.4025979999999993	-2.8696869999999999	-0.1615660000000000
0.0000000000000000	11.3235840000000003	0.0117790000000000
0.0000000000000000	0.0000000000000000	26.8160300000000014

N O Ti

1 3 64

Selective dynamics

Direct

0.2532083527212687	0.4523274120736410	0.4083609247154667
0.3656558190655096	0.4847031006440879	0.3861780498558475
0.1519136751940315	0.4185039462045071	0.3790876837176845
0.2447791522147149	0.4555394717468136	0.4538443509253804
0.0659899999999993	0.0154339999999991	0.0657059999999987
0.1753859907753688	0.1679416886600077	0.1445641946551884
0.2960203942574126	0.0724420744234476	0.2285155234637888
0.4090946594290857	0.2230134128129720	0.3081589203085082
0.2968440000000001	0.1981469999999987	0.0508159999999975
0.4055537011122105	0.1004989934368579	0.1314887261409808
0.0271841732327243	0.0051787192853560	0.2161853024968309
0.1362646685035748	0.1550972834571141	0.2957115417991948
0.5659899999999993	0.0154339999999991	0.0657059999999987
0.6746915372609086	0.1676012807874848	0.1439377411612584
0.7966933033216889	0.0728562640719407	0.2286074977459169
0.9039183555456709	0.2235907190813356	0.3084410505124422
0.7968440000000001	0.1981469999999987	0.0508159999999975
0.9057812063273233	0.1014731930555012	0.1317552565405911
0.5272741748677587	0.0056699474219447	0.2170686661980646
0.6369639463361163	0.1579333779244775	0.2957714488339382

0.065989999999993 0.265433999999991 0.0657059999999987
0.1762540180254077 0.4179640370430729 0.1447037192109070
0.2960473462405405 0.3229611767803364 0.2312271121072550
0.4099658467042564 0.4759050034455158 0.3138805460739335
0.296844000000001 0.4481469999999987 0.0508159999999975
0.4054405445311875 0.3505827795135830 0.1322218823881507
0.0294824939452021 0.2565577646833663 0.2174465625644560
0.1328801314357838 0.4072545948358623 0.3035123392943120
0.565989999999993 0.265433999999991 0.0657059999999987
0.6743605900308363 0.4178862979790344 0.1439420805118860
0.7983540767349174 0.3225371627364063 0.2281451866401383
0.9041366149784709 0.4753286105511773 0.3082312818845651
0.796844000000001 0.4481469999999987 0.0508159999999975
0.9062345003112580 0.3509397309899968 0.1316801321007534
0.5281456591997840 0.2567238976066642 0.2163687271809674
0.6376751971359210 0.4079272547722402 0.2952546803641960
0.065989999999993 0.515433999999991 0.0657059999999987
0.1755708718813882 0.6675125921500997 0.1446275696468688
0.2960409532568152 0.5711002642991100 0.2312399451391047
0.4094047288075410 0.7270887334438302 0.3087698961157936
0.296844000000001 0.6981469999999987 0.0508159999999975
0.4055999366937937 0.6008327827930364 0.1321870170937624

0.0295103405542727 0.5060977722426705 0.2174042544076124
0.1363161347890077 0.6619287896076302 0.2954118314270657
0.5659899999999993 0.5154339999999991 0.0657059999999987
0.6747521082491433 0.6669795778930757 0.1440496268439873
0.7957856249237233 0.5715581658733051 0.2282914646826976
0.9064219065388733 0.7249506320222890 0.3083863190296816
0.7968440000000001 0.6981469999999987 0.0508159999999975
0.9060282085875970 0.6002446902289422 0.1317764148161349
0.5251746992162031 0.5054156783874364 0.2172209222758026
0.6380243366802435 0.6587260200738545 0.2954096157180884
0.0659899999999993 0.7654339999999991 0.0657059999999987
0.1751883845740370 0.9175751453714689 0.1438686180551131
0.2957718965850420 0.8219623603940894 0.2284977103355419
0.4062771458436338 0.9739434419237685 0.3089934070080074
0.2968440000000001 0.9481469999999987 0.0508159999999975
0.4058084154418926 0.8511740176909096 0.1315174163860880
0.0268743295966866 0.7564867670951746 0.2160392680121046
0.1357106727387451 0.9078781501807679 0.2955991944186073
0.5659899999999993 0.7654339999999991 0.0657059999999987
0.6751206603563537 0.9179238864576325 0.1440284698005589
0.7962223129814211 0.8227325075034766 0.2283989914293205
0.9062793969400876 0.9743328665935829 0.3085632758895677

0.7968440000000001 0.9481469999999987 0.0508159999999975
0.9052431266086446 0.8507820190891449 0.1314782947870362
0.5275116162451797 0.7554167691700752 0.2164345611930916
0.6370998843453309 0.9083195057771669 0.2962596080024964

Ti(101)-NO₃H

10.4025979999999993 -2.8696869999999999 -0.1615660000000000
0.0000000000000000 11.3235840000000003 0.0117790000000000
0.0000000000000000 0.0000000000000000 26.8160300000000014

H N O Ti
1 1 3 64

Selective dynamics

Direct

0.2319857466907342 0.4293585527854539 0.4731765917463610
0.2291511664498431 0.4749691625483308 0.4050894517091037
0.3432749119169261 0.4731613975491535 0.3805879807072350
0.1260634062873080 0.4275257722617308 0.3714463738959207
0.2122840686221772 0.3798712567672668 0.4427503395983632
0.0659899999999993 0.0154339999999991 0.0657059999999987
0.1759836069201464 0.1667625024020339 0.1444398119330018
0.2968787625198061 0.0692428064195046 0.2284802549445023
0.4104049385522687 0.2188304254312313 0.3090928477175799

0.296844000000001	0.1981469999999987	0.0508159999999975
0.4062729046252495	0.1004749641550246	0.1316176601214307
0.0276961243239854	0.0033832211083062	0.2158231477399359
0.1375582814314632	0.1514023216573439	0.2958754610939519
0.5659899999999993	0.0154339999999991	0.0657059999999987
0.6754151568304946	0.1667679613004082	0.1444110878266599
0.7951881619430718	0.0687874455069291	0.2281529912390858
0.9031472381913913	0.2153768880021055	0.3084737325331570
0.7968440000000001	0.1981469999999987	0.0508159999999975
0.9060290687495812	0.1007722854507234	0.1315098948901203
0.5272328253985376	0.0033409267973929	0.2171614578360463
0.6375046570920428	0.1546645601594082	0.2958046299326870
0.0659899999999993	0.2654339999999991	0.0657059999999987
0.1762877152026673	0.4165775473169481	0.1452735244247037
0.2967353725404367	0.3190235379611938	0.2312448414424305
0.4042445925197417	0.4712415961586953	0.3154934985392574
0.2968440000000001	0.4481469999999987	0.0508159999999975
0.4060018252375024	0.3502762472871825	0.1324882891669183
0.0292095351000646	0.2526625344687200	0.2171024482741520
0.1303046857350385	0.4033195862034283	0.3010306624108123
0.5659899999999993	0.2654339999999991	0.0657059999999987
0.6746439211952341	0.4165545138041742	0.1442440130257532

0.8004237753161872 0.3203403112268403 0.2294187260835795
0.9032325705613424 0.4738055222451173 0.3085702974166855
0.7968440000000001 0.4481469999999987 0.0508159999999975
0.9063932011972187 0.3505315163435027 0.1317628954485329
0.5298622106957749 0.2553622477240490 0.2170337327033918
0.6369529361366717 0.4044078334622424 0.2960164594262320
0.0659899999999993 0.5154339999999991 0.0657059999999987
0.1757872012735678 0.6660132684162980 0.1444289573672798
0.2973678636512050 0.5691403194082947 0.2310877850283409
0.4106401200152245 0.7237633501640920 0.3092155763181422
0.2968440000000001 0.6981469999999987 0.0508159999999975
0.4058218025248860 0.6000242328676230 0.1321648975140029
0.0293452344774228 0.5066643222836803 0.2176853285482550
0.1373430673102043 0.6613704733304774 0.2964552748236835
0.5659899999999993 0.5154339999999991 0.0657059999999987
0.6746995252128661 0.6650201829814111 0.1440164639168290
0.7935680066466786 0.5679094101180430 0.2285235421683257
0.9058359205896819 0.7207709381136059 0.3078444124480244
0.7968440000000001 0.6981469999999987 0.0508159999999975
0.9058445838087927 0.5996685371415753 0.1319002842546684
0.5245209098556448 0.5030702512614922 0.2182681883694851
0.6372593190989011 0.6564598638078166 0.2958497650015698

0.065989999999993	0.765433999999991	0.065705999999987
0.1757227883960396	0.9162459454940528	0.1440084539836583
0.2954927393913092	0.8184611267882821	0.2285464135674731
0.4062705909542859	0.9694986160286733	0.3090074538794872
0.2968440000000001	0.948146999999987	0.050815999999975
0.4058210000695253	0.8503117745881140	0.1315323817097701
0.0269596070992296	0.7546800397368224	0.2161288707264046
0.1369915818624464	0.9054386109306829	0.2950729259240766
0.565989999999993	0.765433999999991	0.065705999999987
0.6749833610790882	0.9163892375911080	0.1438461784284389
0.7959241910523361	0.8192858294143673	0.2282535967247053
0.9068689572464458	0.9705607388165328	0.3078062183900416
0.7968440000000001	0.948146999999987	0.050815999999975
0.9054154765261315	0.8501376874086052	0.1314904444510688
0.5283420814467705	0.7537281122958890	0.2165937257713570
0.6377074303265259	0.9056676009409869	0.2965348310625978

Ti(101)-NO₂

10.402597999999993	-2.869686999999999	-0.161566000000000
0.000000000000000	11.323584000000003	0.011779000000000
0.000000000000000	0.000000000000000	26.816030000000014

N O Ti

Selective dynamics

Direct

0.2492759385898451	0.4599319445928822	0.4064093601657708
0.3591131490584086	0.4860739239479401	0.3820923693077375
0.1521085825077195	0.4274801501292010	0.3748227293411275
0.0659899999999993	0.0154339999999991	0.0657059999999987
0.1754045853047921	0.1678653870307617	0.1444458390518008
0.2966505654875519	0.0718442914528052	0.2285929124869556
0.4091417802332192	0.2225082202345368	0.3087673670473494
0.2968440000000001	0.1981469999999987	0.0508159999999975
0.4055830629176716	0.1009833114289487	0.1314723838153747
0.0276355262518394	0.0048156890709637	0.2160981971824170
0.1357716804747792	0.1547582421537480	0.2960100555813105
0.5659899999999993	0.0154339999999991	0.0657059999999987
0.6749748952228299	0.1677246964392526	0.1440022369129096
0.7966004106248308	0.0721105715077546	0.2284133635042341
0.9035231827667877	0.2218060854781257	0.3089632758796085
0.7968440000000001	0.1981469999999987	0.0508159999999975
0.9058732392516670	0.1013192412207641	0.1316830901764570
0.5273821691237331	0.0052779885062974	0.2166217709601823
0.6369546448070631	0.1571647017703905	0.2955421572609092

0.065989999999993 0.265433999999991 0.0657059999999987
0.1762184868620308 0.4177900282144498 0.1450179337009744
0.2963526485295199 0.3215143852130031 0.2308026177541316
0.4098137011784164 0.4746630046961182 0.3131669942530177
0.296844000000001 0.4481469999999987 0.0508159999999975
0.4055423058971707 0.3504734834184910 0.1321937747360812
0.0288386349205498 0.2550889659540784 0.2174095179304096
0.1317550789603769 0.4068642885553376 0.3020819465876983
0.565989999999993 0.265433999999991 0.0657059999999987
0.6748271623707561 0.4180204721607259 0.1440675513652054
0.7994394311556573 0.3223092037841989 0.2286635610058923
0.9041928261424524 0.4758075607203585 0.3089143028203641
0.796844000000001 0.4481469999999987 0.0508159999999975
0.9063209834852903 0.3508038881137210 0.1316922289662882
0.5284881400803063 0.2567669066493978 0.2166379252988780
0.6385112945778714 0.4065781671135917 0.2952085217495769
0.065989999999993 0.515433999999991 0.0657059999999987
0.1758747549481085 0.6670173586338313 0.1443999636790667
0.2959032001156360 0.5710286186951726 0.2307500324314110
0.4097212302441861 0.7244710969296115 0.3096077614169345
0.296844000000001 0.6981469999999987 0.0508159999999975
0.4058015889365135 0.6007154371120955 0.1322083750630788

0.0286039339458903	0.5069085217581563	0.2174102255486635
0.1355824805596947	0.6616212439075148	0.2963022977572154
0.5659899999999993	0.5154339999999991	0.0657059999999987
0.6750041071654079	0.6667211289005768	0.1439908431296390
0.7957836013564540	0.5713935386606248	0.2280085336240287
0.9068607263761322	0.7245983918185024	0.3079785487194239
0.7968440000000001	0.6981469999999987	0.0508159999999975
0.9062248605654694	0.6002146980594110	0.1315452958066241
0.5248670748661823	0.5052706701521809	0.2170410678801290
0.6388322502822196	0.6589810070242248	0.2953728623743585
0.0659899999999993	0.7654339999999991	0.0657059999999987
0.1757887835992484	0.9173512057861418	0.1439050511690731
0.2959935669595159	0.8210174845617890	0.2288193493621164
0.4066232886704338	0.9727666316821495	0.3086754756922395
0.2968440000000001	0.9481469999999987	0.0508159999999975
0.4061134673090536	0.8508748691440248	0.1315176576485895
0.0273480778252635	0.7563466065724289	0.2157336894635925
0.1366246692107144	0.9079011554943810	0.2953135526961308
0.5659899999999993	0.7654339999999991	0.0657059999999987
0.6749610580597751	0.9174828853914886	0.1439248805276776
0.7962286604641778	0.8224655867407690	0.2282268243109914
0.9062371625239676	0.9737825999592921	0.3083066460673710

0.7968440000000001 0.9481469999999987 0.0508159999999975
0.9054165832359249 0.8508375510392179 0.1314282675705914
0.5273460513543943 0.7549594007559269 0.2166760884643862
0.6367590473735313 0.9076475106346514 0.2960992782916482

Ti(101)-NO₂H

10.4025979999999993 -2.8696869999999999 -0.1615660000000000
0.0000000000000000 11.3235840000000003 0.0117790000000000
0.0000000000000000 0.0000000000000000 26.8160300000000014

H N O Ti
1 1 2 64

Selective dynamics

Direct

0.2865010000000012 0.4375190000000018 0.4455540000000013
0.3418610000000015 0.4533720000000017 0.3769720000000021
0.2113790000000009 0.4377569999999977 0.3678979999999967
0.3605319999999992 0.4882800000000032 0.4276740000000032
0.0659899999999993 0.0154339999999991 0.0657059999999987
0.1759160000000008 0.1676689999999965 0.1445750000000032
0.2957159999999988 0.0723300000000009 0.2296830000000014
0.4137970000000024 0.2283499999999989 0.3094600000000014
0.2968440000000001 0.1981469999999987 0.0508159999999975

0.4051240000000007	0.1003499999999988	0.1314700000000002
0.0289720000000031	0.0054659999999984	0.2178979999999981
0.1412899999999979	0.1574239999999989	0.2974350000000001
0.5659899999999993	0.0154339999999991	0.0657059999999987
0.6754480000000029	0.1670349999999985	0.1434670000000011
0.7958270000000027	0.0705209999999994	0.2282500000000027
0.9087949999999978	0.2221219999999988	0.3076160000000030
0.7968440000000001	0.1981469999999987	0.0508159999999975
0.9070239999999998	0.1011600000000001	0.1321209999999979
0.5265190000000004	0.0023259999999965	0.2158579999999972
0.6387369999999990	0.1511599999999973	0.2949210000000022
0.0659899999999993	0.2654339999999991	0.0657059999999987
0.1761199999999974	0.4173309999999972	0.1445739999999986
0.3001069999999970	0.3205540000000013	0.2315759999999969
0.4089870000000033	0.4816920000000025	0.3208339999999978
0.2968440000000001	0.4481469999999987	0.0508159999999975
0.4066499999999991	0.3515790000000010	0.1323080000000019
0.0330489999999983	0.2553100000000015	0.2173590000000019
0.1376009999999965	0.4088849999999979	0.3019940000000005
0.5659899999999993	0.2654339999999991	0.0657059999999987
0.6745099999999979	0.4184339999999978	0.1461200000000034
0.8024449999999987	0.3200720000000032	0.2277940000000029

0.908768999999995	0.474097000000004	0.3093379999999968
0.7968440000000001	0.4481469999999987	0.0508159999999975
0.9062550000000016	0.3506399999999985	0.1313189999999977
0.5305650000000028	0.2508499999999998	0.2158810000000031
0.6431210000000007	0.3996029999999990	0.2936240000000012
0.0659899999999993	0.5154339999999991	0.0657059999999987
0.1749310000000008	0.6670280000000020	0.1440610000000007
0.2944430000000011	0.5727619999999973	0.2292059999999978
0.4066940000000017	0.7248069999999984	0.3071709999999968
0.2968440000000001	0.6981469999999987	0.0508159999999975
0.4065760000000012	0.5997559999999993	0.1317370000000011
0.0283220000000028	0.5062479999999994	0.2166750000000022
0.1377740000000003	0.6559859999999986	0.2965689999999981
0.5659899999999993	0.5154339999999991	0.0657059999999987
0.6745730000000023	0.6655659999999983	0.1445250000000016
0.7960380000000029	0.5727720000000005	0.2295599999999993
0.9090630000000033	0.7276710000000008	0.3075260000000029
0.7968440000000001	0.6981469999999987	0.0508159999999975
0.9044960000000017	0.5999839999999992	0.1319739999999996
0.5233160000000012	0.5063719999999989	0.2215569999999971
0.6367690000000010	0.6606409999999983	0.2978400000000008
0.0659899999999993	0.7654339999999991	0.0657059999999987

0.174923999999972	0.917805000000013	0.144390999999988
0.294918000000027	0.822020999999994	0.228619999999994
0.406512999999968	0.975754000000020	0.308050999999990
0.296844000000001	0.948146999999987	0.050815999999975
0.405253000000019	0.850152999999988	0.131414999999970
0.028514000000013	0.755040999999985	0.216461000000025
0.137073000000009	0.907237999999995	0.296920000000030
0.565989999999993	0.765433999999991	0.065705999999987
0.675736999999980	0.916860999999973	0.143569999999969
0.796723999999975	0.821886999999967	0.228628000000005
0.905773000000035	0.974487000000034	0.309339999999988
0.796844000000001	0.948146999999987	0.050815999999975
0.906165999999989	0.850704999999978	0.131616999999985
0.528519000000028	0.755549999999995	0.215857999999972
0.637385000000019	0.906171999999980	0.295504000000011

Ti(101)-NO

10.402597999999993	-2.869686999999999	-0.161566000000000
0.000000000000000	11.323584000000003	0.011779000000000
0.000000000000000	0.000000000000000	26.816030000000014

N O Ti

1 1 64

Selective dynamics

Direct

0.3185160000000025	0.5136400000000023	0.3437249999999992
0.1891820000000024	0.5343840000000029	0.3485500000000030
0.0659899999999993	0.0154339999999991	0.0657059999999987
0.1753679999999989	0.1674250000000015	0.1445310000000006
0.2946779999999976	0.0715620000000001	0.2288649999999990
0.4020439999999965	0.2192509999999999	0.3097319999999968
0.2968440000000001	0.1981469999999987	0.0508159999999975
0.4059629999999999	0.1005800000000008	0.1317599999999999
0.0265470000000008	0.0043340000000001	0.2169930000000022
0.1360060000000018	0.1562720000000013	0.2959660000000000
0.5659899999999993	0.0154339999999991	0.0657059999999987
0.6752269999999996	0.1668639999999968	0.1442639999999997
0.7960119999999975	0.0722239999999985	0.2293009999999995
0.9078760000000017	0.2235289999999992	0.3078730000000007
0.7968440000000001	0.1981469999999987	0.0508159999999975
0.9058890000000019	0.1004220000000018	0.1316539999999975
0.5283129999999971	0.0036229999999975	0.2170899999999989
0.6356830000000002	0.1548820000000006	0.2981639999999999
0.0659899999999993	0.2654339999999991	0.0657059999999987
0.1746130000000008	0.4177830000000000	0.1444949999999992

0.2987219999999979 0.3210649999999973 0.2312879999999993
0.4087839999999971 0.4810829999999982 0.3160069999999990
0.2968440000000001 0.4481469999999987 0.0508159999999975
0.4054780000000022 0.3504659999999973 0.1320419999999984
0.0296510000000012 0.2558030000000002 0.2164169999999999
0.1334599999999995 0.4083380000000005 0.2987809999999982
0.5659899999999993 0.2654339999999991 0.0657059999999987
0.6752099999999999 0.4172700000000020 0.1453479999999985
0.7974979999999974 0.3212079999999986 0.2301670000000016
0.8994069999999965 0.4754069999999970 0.3117170000000016
0.7968440000000001 0.4481469999999987 0.0508159999999975
0.9052349999999976 0.3505600000000015 0.1318699999999993
0.5275930000000003 0.2516490000000005 0.2172020000000003
0.6341520000000003 0.4036230000000032 0.2978000000000023
0.0659899999999993 0.5154339999999991 0.0657059999999987
0.1735159999999993 0.6668110000000027 0.1440049999999999
0.2915789999999987 0.5715280000000007 0.2287869999999970
0.4037870000000012 0.7274790000000024 0.3075100000000006
0.2968440000000001 0.6981469999999987 0.0508159999999975
0.4049550000000011 0.6005529999999979 0.1317609999999974
0.0230729999999966 0.5056930000000008 0.2176800000000014
0.1343480000000028 0.6558679999999981 0.2993280000000027

0.565989999999993 0.515433999999991 0.0657059999999987
0.674542999999999 0.6675830000000005 0.1440070000000020
0.7938350000000014 0.5729309999999970 0.2302650000000028
0.907209999999992 0.7283400000000029 0.3080849999999984
0.7968440000000001 0.6981469999999987 0.0508159999999975
0.9048179999999988 0.6003860000000003 0.1317889999999977
0.5258249999999975 0.5085890000000006 0.2164149999999978
0.6328010000000006 0.6580709999999996 0.3000219999999985
0.065989999999993 0.765433999999991 0.0657059999999987
0.1741560000000035 0.9173380000000009 0.1439850000000007
0.2933620000000019 0.8217300000000023 0.2280019999999965
0.4055409999999995 0.9739980000000017 0.3078160000000025
0.2968440000000001 0.9481469999999987 0.0508159999999975
0.4058479999999989 0.8505359999999982 0.1316720000000018
0.0259250000000009 0.7548770000000005 0.2163139999999970
0.1369299999999996 0.9082509999999999 0.2962509999999980
0.565989999999993 0.765433999999991 0.0657059999999987
0.6751700000000014 0.9172599999999989 0.1443080000000023
0.7932070000000024 0.8212260000000029 0.2293540000000007
0.9064529999999991 0.9740439999999992 0.3099490000000031
0.7968440000000001 0.9481469999999987 0.0508159999999975
0.9054900000000004 0.8506679999999989 0.1315110000000033

0.5273800000000008 0.7549250000000001 0.2173840000000027

0.63883400000000028 0.9070979999999977 0.2969799999999978

Ti(101)-NHO

10.4025979999999993 -2.8696869999999999 -0.1615660000000000

0.0000000000000000 11.3235840000000003 0.0117790000000000

0.0000000000000000 0.0000000000000000 26.8160300000000014

H N O Ti

1 1 1 64

Selective dynamics

Direct

0.3306609999999992 0.4569729999999979 0.3883900000000011

0.3116380000000021 0.4811180000000022 0.3533279999999976

0.2015079999999969 0.537999999999967 0.3453549999999979

0.0659899999999993 0.0154339999999991 0.0657059999999987

0.1755339999999990 0.1675260000000023 0.1444880000000026

0.2948450000000022 0.0703639999999979 0.2283830000000009

0.4007399999999990 0.2188250000000025 0.3077279999999973

0.2968440000000001 0.1981469999999987 0.0508159999999975

0.4056939999999969 0.1006029999999996 0.1315310000000025

0.0268680000000003 0.0048730000000035 0.2172780000000003

0.1361849999999976 0.1566410000000005 0.2957480000000032

0.565989999999993	0.015433999999991	0.065705999999987
0.6753610000000023	0.167175999999978	0.144041999999989
0.7965080000000029	0.073569999999966	0.2287230000000022
0.9065930000000009	0.225425999999988	0.3070480000000018
0.7968440000000001	0.198146999999987	0.050815999999975
0.906233999999978	0.100495999999997	0.1317030000000017
0.5279510000000016	0.0034940000000034	0.2166250000000005
0.6366190000000032	0.153145999999996	0.296565999999986
0.065989999999993	0.265433999999991	0.065705999999987
0.1744950000000003	0.417600999999977	0.1444350000000014
0.298290999999990	0.320273999999977	0.230505999999983
0.409951999999970	0.4771870000000007	0.314849999999999
0.2968440000000001	0.448146999999987	0.050815999999975
0.4056160000000020	0.3510070000000027	0.132032999999998
0.0294390000000035	0.2568910000000031	0.2166300000000021
0.1347530000000035	0.4086380000000034	0.2965090000000004
0.565989999999993	0.265433999999991	0.065705999999987
0.674684999999966	0.418028999999971	0.144987999999979
0.7957760000000036	0.322868999999972	0.2297650000000004
0.901868999999978	0.4756270000000029	0.3104680000000002
0.7968440000000001	0.448146999999987	0.050815999999975
0.9055600000000013	0.350760999999985	0.131895999999976

0.528398000000028	0.252595999999969	0.216673999999976
0.636037999999992	0.401355000000023	0.300052999999983
0.065989999999993	0.515433999999991	0.065705999999987
0.173898999999987	0.666684000000036	0.144140000000002
0.292923999999993	0.570703000000017	0.229374999999974
0.404558999999990	0.724910000000013	0.307411000000019
0.296844000000001	0.698146999999987	0.050815999999975
0.405113999999975	0.600025000000023	0.132055999999986
0.024309000000024	0.505980999999985	0.217874999999994
0.136080999999972	0.656880999999985	0.296615000000027
0.565989999999993	0.515433999999991	0.065705999999987
0.674227999999994	0.667068000000004	0.144452999999986
0.793539000000027	0.572395999999977	0.231011999999998
0.907809000000003	0.730010000000000	0.307549000000016
0.796844000000001	0.698146999999987	0.050815999999975
0.904707000000019	0.600316999999969	0.132227999999978
0.526212999999985	0.507083999999990	0.218251000000022
0.635280999999991	0.662917000000002	0.297266999999979
0.065989999999993	0.765433999999991	0.065705999999987
0.174196999999995	0.917279999999981	0.143988000000002
0.293736000000027	0.820824999999992	0.228194999999995
0.405087999999992	0.972831999999968	0.307605000000023

0.2968440000000001	0.9481469999999987	0.0508159999999975
0.4054909999999978	0.8506739999999979	0.1315570000000008
0.0270280000000014	0.7546400000000020	0.2164539999999988
0.13689200000000031	0.9087269999999990	0.2964419999999990
0.5659899999999993	0.7654339999999991	0.0657059999999987
0.67543400000000028	0.91737100000000028	0.1439620000000019
0.79440900000000017	0.82245700000000000	0.22853700000000029
0.90621800000000026	0.9756989999999988	0.30996600000000029
0.79684400000000001	0.9481469999999987	0.0508159999999975
0.9055609999999987	0.85061100000000007	0.1314089999999979
0.5270099999999971	0.75557200000000008	0.2166799999999967
0.6382589999999979	0.90683700000000030	0.29592800000000035

Ti(101)-NH₂O

10.4025979999999993	-2.8696869999999999	-0.16156600000000000
0.00000000000000000	11.32358400000000003	0.01177900000000000
0.00000000000000000	0.00000000000000000	26.81603000000000014

H	N	O	Ti
2	1	1	64

Selective dynamics

Direct

0.26934399999999967	0.41637599999999996	0.37998499999999978
---------------------	---------------------	---------------------

0.363422999999974 0.562117999999981 0.383547000000001
0.304654999999968 0.496963999999984 0.360987000000015
0.198666000000029 0.543621999999992 0.345610999999981
0.065989999999993 0.015433999999991 0.065705999999987
0.174757999999971 0.167425000000015 0.144148999999988
0.293813999999976 0.069729000000024 0.227594000000034
0.401536000000001 0.219191000000021 0.304853999999988
0.296844000000001 0.198146999999987 0.050815999999975
0.404921999999991 0.100628999999979 0.131202000000018
0.025728000000009 0.005149000000030 0.217241999999988
0.135731999999973 0.156647999999970 0.295445999999983
0.565989999999993 0.015433999999991 0.065705999999987
0.674916000000032 0.166657000000007 0.144025999999967
0.795639999999988 0.072217000000020 0.228310999999979
0.905684999999983 0.224913000000008 0.306930999999987
0.796844000000001 0.198146999999987 0.050815999999975
0.905437999999966 0.100560000000015 0.131599000000014
0.525723999999967 0.003495000000009 0.216447000000023
0.636400000000019 0.153961999999999 0.294902000000004
0.065989999999993 0.265433999999991 0.065705999999987
0.174227999999994 0.417287999999992 0.143889000000015
0.295991000000008 0.320435000000034 0.228897000000035

0.4102749999999986 0.4742829999999998 0.3140110000000007
0.2968440000000001 0.4481469999999987 0.0508159999999975
0.4052700000000016 0.3514479999999978 0.1316559999999996
0.0278139999999993 0.2570819999999969 0.2164130000000029
0.1379549999999981 0.4086130000000026 0.2961669999999970
0.5659899999999993 0.2654339999999991 0.0657059999999987
0.6743809999999968 0.4181359999999970 0.1442970000000017
0.7954489999999979 0.3235829999999993 0.2286969999999968
0.9076129999999978 0.4753210000000010 0.3075970000000012
0.7968440000000001 0.4481469999999987 0.0508159999999975
0.9052179999999979 0.3507710000000017 0.1314479999999989
0.5285119999999992 0.2548340000000024 0.2156260000000003
0.6383769999999984 0.4017270000000011 0.3005750000000020
0.0659899999999993 0.5154339999999991 0.0657059999999987
0.1742320000000035 0.6673639999999992 0.1439919999999972
0.2951910000000026 0.5711930000000009 0.2290720000000022
0.4047320000000028 0.7231220000000036 0.3075120000000027
0.2968440000000001 0.6981469999999987 0.0508159999999975
0.4053320000000014 0.6000909999999990 0.1318079999999995
0.0270920000000032 0.5065329999999975 0.2164750000000026
0.1380709999999965 0.6577399999999969 0.2962119999999970
0.5659899999999993 0.5154339999999991 0.0657059999999987

0.6740580000000023 0.6669740000000033 0.1443370000000002
0.7929219999999972 0.5708569999999966 0.2302359999999979
0.9067020000000028 0.7263030000000015 0.3073699999999988
0.7968440000000001 0.6981469999999987 0.0508159999999975
0.9045180000000030 0.6005880000000019 0.1320509999999970
0.5271499999999989 0.5051440000000014 0.2187959999999975
0.6372539999999987 0.6635109999999997 0.2961159999999978
0.0659899999999993 0.7654339999999991 0.0657059999999987
0.1736300000000028 0.9172790000000006 0.1438909999999964
0.2941969999999969 0.8206160000000011 0.2285010000000014
0.4049499999999995 0.9738010000000017 0.3083260000000010
0.2968440000000001 0.9481469999999987 0.0508159999999975
0.4049309999999977 0.8506920000000022 0.1315650000000019
0.0271359999999987 0.7547560000000004 0.2164720000000031
0.1361119999999971 0.9086720000000028 0.2962830000000025
0.5659899999999993 0.7654339999999991 0.0657059999999987
0.6748910000000024 0.9172849999999997 0.1439140000000023
0.7948549999999983 0.8217890000000025 0.2286270000000030
0.9049029999999973 0.9744239999999991 0.3097860000000026
0.7968440000000001 0.9481469999999987 0.0508159999999975
0.9050859999999972 0.8506360000000015 0.1313850000000016
0.5274379999999965 0.7557729999999978 0.2166229999999985

0.6361240000000024 0.9067390000000017 0.2958179999999970

Ti(101)-O

10.4025979999999993 -2.8696869999999999 -0.1615660000000000

0.0000000000000000 11.3235840000000003 0.0117790000000000

0.0000000000000000 0.0000000000000000 26.8160300000000014

O Ti

1 64

Selective dynamics

Direct

0.2713249999999974 0.5646920000000009 0.3165130000000005

0.0659899999999993 0.0154339999999991 0.0657059999999987

0.1741290000000006 0.1665800000000033 0.1441090000000003

0.2953830000000011 0.0704279999999997 0.2291129999999981

0.4066839999999985 0.2222579999999965 0.3091110000000015

0.2968440000000001 0.1981469999999987 0.0508159999999975

0.4049520000000015 0.1002579999999966 0.1317700000000031

0.0272569999999988 0.0043900000000008 0.2168229999999980

0.1350649999999973 0.1573599999999971 0.2967330000000032

0.5659899999999993 0.0154339999999991 0.0657059999999987

0.6744500000000002 0.1665279999999996 0.1442410000000010

0.7951830000000015 0.0696089999999998 0.2289979999999971

0.904049999999980	0.220937999999967	0.309252000000007
0.796844000000001	0.198146999999987	0.050815999999975
0.904505999999978	0.099814000000021	0.131759999999999
0.526366000000030	0.003804999999998	0.217511000000018
0.636316999999982	0.157096000000028	0.296729999999966
0.065989999999993	0.265433999999991	0.065705999999987
0.175539999999980	0.417498000000019	0.144683999999980
0.294367999999986	0.319026000000009	0.229084000000003
0.406064000000006	0.469065000000005	0.308680000000025
0.296844000000001	0.448146999999987	0.050815999999975
0.404769000000017	0.349701000000031	0.131431999999967
0.025072999999990	0.252845000000007	0.216726999999988
0.134413000000021	0.406210000000015	0.296911999999990
0.565989999999993	0.265433999999991	0.065705999999987
0.674517000000016	0.416482000000020	0.144128000000020
0.795290000000014	0.319476999999991	0.228914000000032
0.904251000000021	0.472251999999975	0.307639999999992
0.796844000000001	0.448146999999987	0.050815999999975
0.905071999999970	0.349997000000019	0.131590000000028
0.526460000000002	0.254759999999974	0.217204999999999
0.637070999999988	0.406891999999991	0.296456999999966
0.065989999999993	0.515433999999991	0.065705999999987

0.1753130000000027 0.6664800000000000 0.1446529999999981
0.2940540000000027 0.5703699999999969 0.2300030000000035
0.4063659999999985 0.7279550000000015 0.3086890000000011
0.2968440000000001 0.6981469999999987 0.0508159999999975
0.4050670000000025 0.6005430000000018 0.1317090000000007
0.0247919999999979 0.5040219999999991 0.2158439999999970
0.1344629999999967 0.6550429999999992 0.2971130000000031
0.5659899999999993 0.5154339999999991 0.0657059999999987
0.6742440000000016 0.6665240000000026 0.1440800000000024
0.7940770000000015 0.5698829999999973 0.2284930000000003
0.9023150000000015 0.7219550000000012 0.3090509999999966
0.7968440000000001 0.6981469999999987 0.0508159999999975
0.9052089999999993 0.6004149999999981 0.1314640000000011
0.5247919999999979 0.5040660000000017 0.2159270000000006
0.6336310000000012 0.6557159999999982 0.2953660000000013
0.0659899999999993 0.7654339999999991 0.0657059999999987
0.1740080000000006 0.9165909999999968 0.1440979999999996
0.2931340000000020 0.8212100000000007 0.2290980000000005
0.4065569999999994 0.9738710000000026 0.3091170000000005
0.2968440000000001 0.9481469999999987 0.0508159999999975
0.4046319999999994 0.8509669999999971 0.1315570000000008
0.0242089999999990 0.7545479999999998 0.2167880000000011

0.134799000000010	0.904020000000027	0.296917999999980
0.565989999999993	0.765433999999991	0.065705999999987
0.673687000000010	0.916516999999989	0.144039999999968
0.794136000000017	0.820782000000012	0.228611000000008
0.906537000000001	0.972026999999971	0.308402999999984
0.796844000000001	0.948146999999987	0.050815999999975
0.904755999999990	0.850498000000018	0.131639999999973
0.524633999999989	0.754624999999972	0.216166000000012
0.638483999999983	0.907412999999982	0.296944000000034

Ti(101)-OH

10.402597999999993	-2.869686999999999	-0.161566000000000
0.000000000000000	11.323584000000003	0.011779000000000
0.000000000000000	0.000000000000000	26.816030000000014

H	O	Ti
1	1	64

Selective dynamics

Direct

0.252242000000025	0.557791000000017	0.382404000000011
0.264158999999994	0.561593000000020	0.346241999999966
0.065989999999993	0.015433999999991	0.065705999999987
0.174548000000015	0.166635999999969	0.144522999999995

0.2971470000000025	0.0702179999999970	0.2296350000000018
0.4057069999999996	0.2243640000000013	0.3090959999999967
0.2968440000000001	0.1981469999999987	0.0508159999999975
0.4050319999999985	0.1002239999999972	0.1320260000000033
0.0286290000000022	0.0047240000000031	0.2176079999999985
0.1359100000000026	0.1583749999999995	0.2971020000000024
0.5659899999999993	0.0154339999999991	0.0657059999999987
0.6746359999999996	0.1665380000000027	0.1442180000000022
0.7967220000000026	0.0705030000000022	0.2294819999999973
0.9055409999999995	0.2240129999999994	0.3093900000000005
0.7968440000000001	0.1981469999999987	0.0508159999999975
0.9054539999999989	0.1006470000000022	0.1320920000000001
0.5279809999999969	0.0039530000000028	0.2175780000000032
0.6351769999999988	0.1561990000000009	0.2968010000000021
0.0659899999999993	0.2654339999999991	0.0657059999999987
0.1738029999999995	0.4166590000000028	0.1433370000000025
0.2939590000000010	0.3199900000000028	0.2295069999999981
0.4029179999999997	0.4749729999999985	0.3084980000000002
0.2968440000000001	0.4481469999999987	0.0508159999999975
0.4047010000000029	0.3508270000000024	0.1321879999999993
0.0267910000000029	0.2558030000000002	0.2175700000000020
0.1369100000000003	0.4085469999999987	0.2988860000000031

0.565989999999993	0.265433999999991	0.065705999999987
0.673875999999999	0.416792999999984	0.144229000000028
0.794927000000013	0.320154999999997	0.228805999999987
0.905279000000002	0.473339000000028	0.307074999999975
0.796844000000001	0.448146999999987	0.050815999999975
0.904985000000035	0.350400000000005	0.131833000000003
0.526718999999999	0.254994000000035	0.217506000000002
0.636217999999995	0.406309999999977	0.296875999999975
0.065989999999993	0.515433999999991	0.065705999999987
0.173861000000023	0.666488999999986	0.143436000000012
0.296492000000006	0.570610999999995	0.224291000000009
0.403258000000010	0.717011999999969	0.308264999999987
0.296844000000001	0.698146999999987	0.050815999999975
0.406283000000019	0.600704000000003	0.130375999999983
0.027579000000029	0.505383000000019	0.216858000000020
0.137166000000006	0.655360000000017	0.299235000000030
0.565989999999993	0.515433999999991	0.065705999999987
0.675123999999967	0.666882999999986	0.143940000000006
0.793778000000032	0.570408999999979	0.228827000000026
0.906235000000023	0.721825000000026	0.309201999999991
0.796844000000001	0.698146999999987	0.050815999999975
0.905324999999977	0.600441000000036	0.131892000000006

0.5266370000000009	0.5045059999999992	0.2174570000000031
0.6359399999999980	0.6558700000000002	0.2974430000000012
0.0659899999999993	0.7654339999999991	0.0657059999999987
0.1745710000000003	0.9164669999999973	0.1444940000000017
0.2939689999999970	0.8192000000000021	0.2295519999999982
0.4065939999999983	0.9693929999999966	0.3090070000000011
0.2968440000000001	0.9481469999999987	0.0508159999999975
0.4052530000000019	0.8498239999999981	0.1321909999999988
0.0270429999999990	0.7536690000000021	0.2176869999999980
0.1372270000000029	0.9054289999999980	0.2973380000000034
0.5659899999999993	0.7654339999999991	0.0657059999999987
0.6744330000000005	0.9165009999999967	0.1443859999999972
0.7952470000000034	0.8206909999999965	0.2294669999999996
0.9071330000000017	0.9725389999999976	0.3089810000000028
0.7968440000000001	0.9481469999999987	0.0508159999999975
0.9059949999999972	0.8503729999999976	0.1321719999999971
0.5273380000000003	0.7545300000000026	0.2174669999999992
0.6373940000000005	0.9063749999999970	0.2971429999999984

TiH_{1.97}-NO₃

10.1930359999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000

0.0000000000000000 0.0000000000000000 27.2903899999999986

H N O Ti

96 1 3 48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4036845653044761	0.0138307772470372	0.1238387005481414
0.2325443017214855	0.1723653361001257	0.2226721100136143
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3195079481984787	0.0963850865960851	0.1813975344047735
0.1536428640948035	0.2632151651725007	0.2847335256420035
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4041879027681285	0.2646678280209855	0.1239077196343038
0.2376538286544806	0.4339579201170792	0.2257102710246033
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3193933660771438	0.3464407091225798	0.1798973383805180
0.1525350040211904	0.0135360369390559	0.2859257885014919
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1540714917959495	0.2646235193273352	0.1239095008318213
0.4888156334626286	0.4338904208244288	0.2257244535671054
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0698513481082522	0.3476911962995389	0.1818780054810959

0.4035496836417307	0.0150531204113306	0.2857229180873683
0.3205450000000027	0.346559999999966	0.0195900000000009
0.1531124401996401	0.0125992361230349	0.1238173623638696
0.4858255998207182	0.1803397158137554	0.2239698644769010
0.2367330000000010	0.4300550000000030	0.0814719999999980
0.0692993382236018	0.0963411005853909	0.1813867417043137
0.4010684589629230	0.2631135199104510	0.2847379495002826
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.9037591860287632	0.0138653461985488	0.1238308130283735
0.7371383558244956	0.1818029675170810	0.2241375642490616
0.9867330000000010	0.4300550000000030	0.0814719999999980
0.8203967980756400	0.0981383165568540	0.1815223830590105
0.6533454689736842	0.2649485470441150	0.2861423384025236
0.5705460000000002	0.096559999999966	0.0195900000000009
0.9039416281680348	0.2641386805741846	0.1238577530767203
0.7368868623066047	0.4309127710696301	0.2244031686359409
0.9867330000000010	0.1800550000000030	0.0814719999999980
0.8200102072299735	0.3477226768277601	0.1818918309029075
0.6540923750480687	0.0166598093830786	0.2851376664640816
0.8205460000000002	0.096559999999966	0.0195900000000009
0.6538210342931865	0.2642221783741477	0.1238603483542312
0.9864285251104873	0.4308865098529052	0.2244135695590884

0.736733000000010	0.180053999999984	0.081471999999980
0.5701711865473393	0.3477090725681569	0.1818750913081408
0.9030706790305186	0.0150099662980687	0.2856748778519252
0.820546000000002	0.346559999999966	0.019590000000009
0.6539498280935871	0.0142731576386255	0.1237716015462872
0.9871185140550119	0.1803425468944108	0.2239771230731084
0.736733000000010	0.430055000000030	0.081471999999980
0.5701004315395405	0.0981620674470325	0.1815342530954693
0.9031490217441027	0.2650612536184714	0.2861056678262896
0.070546000000002	0.846561000000012	0.019590000000009
0.4036631295400089	0.5138375742019182	0.1243268467556025
0.2396904918346290	0.6794987286927880	0.2264183707289373
0.486733000000010	0.930055000000030	0.081471999999980
0.3202273142116314	0.5968887747352325	0.1837632989679882
0.1535545926669349	0.7648175846623125	0.2856115531742994
0.070546000000002	0.596561000000012	0.019590000000009
0.4042042830473734	0.7631061186929645	0.1243474953180923
0.2350850715789898	0.9311443625613967	0.2236096374995220
0.486733000000010	0.680053999999984	0.081471999999980
0.3201698754182422	0.8474229685559025	0.1814723711954530
0.1433215956100615	0.5095081121094123	0.2864350212994692
0.320545000000027	0.596561000000012	0.019590000000009

0.1537811886322179 0.7625026129756186 0.1240995799189261
0.4865674325625071 0.9342444558250743 0.2234717309026616
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0696908920372799 0.8469303665369365 0.1816891278563992
0.3934580669242577 0.4953068275199690 0.2769777672658557
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1536915932654867 0.5140029539360724 0.1240497251924110
0.4859856290403438 0.6794599055520865 0.2288507612814807
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0704393841390585 0.5973345774709522 0.1820241535526420
0.4101732077309018 0.7813101789408077 0.2832014323316936
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9035389254540894 0.5135075769761889 0.1238805147237045
0.7324126907332706 0.6793924649062388 0.2263803931260525
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8193098851438676 0.5974372735132082 0.1820492268182273
0.6625654523547776 0.7811758500737589 0.2830868460852043
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9023393822193675 0.7624776339470160 0.1240927743483570
0.7402540699484421 0.9342017542893194 0.2234801315521903
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8196510291110433 0.8473762993385388 0.1814647232374648

0.6575918733635739	0.5093707939969725	0.2864797807889168
0.8205460000000002	0.5965610000000012	0.0195900000000009
0.6524339284014574	0.7630718251136758	0.1243259419896991
0.9887297632876578	0.9310401969850154	0.2236214985104149
0.7367330000000010	0.6800550000000030	0.0814719999999980
0.5699764407285536	0.8475824194777374	0.1811553451742582
0.9033533193651916	0.5150328801783176	0.2854079212788760
0.8205460000000002	0.8465610000000012	0.0195900000000009
0.6538384972665633	0.5140151232790622	0.1240792396043634
0.9865799713939312	0.6807254419092261	0.2244358028557402
0.7367330000000010	0.9300550000000030	0.0814719999999980
0.5689909785418246	0.5969480296989553	0.1837623782121944
0.9029855934389709	0.7648422096467699	0.2855752119973340
0.4467072946197342	0.6017006036158541	0.3597509519454234
0.5422280124314053	0.6021247059423639	0.3354509784324283
0.3516425251205976	0.6020007069598620	0.3354600227509558
0.4455406442046266	0.5998091917601290	0.4045851701893065
0.4036389999999983	0.2633080000000021	0.0542870000000022
0.2370853256816021	0.4322046432502473	0.1534579742477311
0.0688843959995625	0.0960526972675636	0.2512538997644580
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.2362638426186603	0.1794222578472156	0.1521810372104450

0.0686521587239026	0.3461516212702136	0.2512210211524877
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4868326251932196	0.1808178955586908	0.1526739640729612
0.3151623745673162	0.3384560988994918	0.2477099676192938
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.4880301055763752	0.4322852612745363	0.1534682596634546
0.3192771359697674	0.0960729808676743	0.2512833093440596
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7367825648532617	0.4308744482793813	0.1530421458504818
0.5705699242191425	0.1000974304090764	0.2512933066910258
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7370683971234094	0.1812500543733920	0.1527130430294634
0.5695354428975915	0.3461066963014555	0.2512484351905281
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9869837786656934	0.1807810722659646	0.1527036758210315
0.8196655600892222	0.3475352926361790	0.2515339215386888
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9869527694423323	0.4307667488120761	0.1530036762883931
0.8215742129422892	0.1001827283190965	0.2512693824542295
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2365408164556479	0.9298128627613986	0.1526677370301648
0.0704158246792893	0.5981870475255968	0.2513468080274921

0.403638999999983	0.513308000000021	0.054287000000022
0.2377288242585462	0.6797128329612848	0.1536750323258507
0.0699081074112035	0.8475383196383736	0.2514279473358337
0.153638999999983	0.513308000000021	0.054287000000022
0.4857388164832568	0.6785726576697364	0.1545909146573206
0.3192502181263724	0.8502196016038706	0.2505306675580123
0.153638999999983	0.763308000000021	0.054287000000022
0.4871315698026423	0.9309320831674023	0.1526387219595474
0.3209588830811571	0.5983916858190261	0.2598899912673964
0.903638999999983	0.763308000000021	0.054287000000022
0.7368188075188367	0.9308326468392483	0.1526289202925756
0.5695549760326331	0.5982932469289444	0.2597298645230306
0.903638999999983	0.513308000000021	0.054287000000022
0.7349709923274708	0.6797691820274538	0.1536368967704976
0.5728161740290579	0.8537157168237540	0.2495505799089913
0.653638999999983	0.513308000000021	0.054287000000022
0.9865070798018444	0.6799627371294064	0.1529087108919054
0.8229434249998854	0.8500348925728447	0.2505086687368674
0.653638999999983	0.763308000000021	0.054287000000022
0.9862306554692853	0.9297742358705108	0.1526426264229594
0.8196270070667591	0.5980610022759555	0.2514037576853025

TiH_{1.97}-Hv-NO₃H

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H	N	O	Ti
96	1	3	48

Selective dynamics

Direct

0.070546000000002	0.346561000000012	0.019590000000009
0.4045947802132775	0.0138358621725562	0.1238805119868844
0.2422211210405698	0.1914732190824102	0.2272167975362564
0.486733000000010	0.430055000000030	0.081471999999980
0.3201183123655064	0.0989299022525679	0.1818905118750978
0.1416530858899616	0.2568684914008053	0.2846801823644279
0.070546000000002	0.096559999999966	0.019590000000009
0.4041807987073970	0.2651009538198281	0.1242120024086441
0.2346317275955346	0.4286024941482208	0.2254099050200535
0.486733000000010	0.180055000000030	0.081471999999980
0.3215799659313636	0.3508218703235418	0.1855463741370887
0.1540345842863362	0.0159344019896293	0.2861076435828031
0.320545000000027	0.096559999999966	0.019590000000009
0.1543212014553468	0.2650604784614978	0.1241803460264540

0.4867249592931256 0.4286485947042976 0.2253766180248324
0.2367330000000010 0.1800539999999984 0.0814719999999980
0.0691114083213841 0.3468716677950117 0.1815044017864718
0.4022801247449480 0.0139901378176461 0.2855134329208865
0.3205450000000027 0.3465599999999966 0.0195900000000009
0.1553315920868193 0.0169015273670306 0.1241137110835733
0.4860436763701128 0.1776729215108000 0.2237302546577257
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0711792788452712 0.0989785844232830 0.1819717068973722
0.4069546483423059 0.2567030046626921 0.2845138816316478
0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9030724647567013 0.0139376746274630 0.1238350707072488
0.7359429877205382 0.1793705141024796 0.2242265888671085
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8192714970140752 0.0962905220158153 0.1817519063345989
0.6546158317242895 0.2616781505204057 0.2863055015932483
0.5705460000000002 0.0965599999999966 0.0195900000000009
0.9030569165615012 0.2628675912875105 0.1237307535608689
0.7401414261784536 0.4315650146774483 0.2229120012115106
0.9867330000000010 0.1800550000000030 0.0814719999999980
0.8195123795010032 0.3465119484854789 0.1811756315157651
0.6513168077025203 0.0111783604435369 0.2859365608945695

0.8205460000000002	0.0965599999999966	0.0195900000000009
0.6533416919496011	0.2629154746848502	0.1237369838799188
0.9844096095496283	0.4316215015363690	0.2229239354949809
0.7367330000000010	0.1800539999999984	0.0814719999999980
0.5703621807327889	0.3470199105671642	0.1814314889563325
0.9034293729367325	0.0140504624725825	0.2854209100040730
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6531907459977667	0.0127968910712758	0.1238234627929095
0.9843076241385526	0.1775537310722196	0.2237803352005018
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5693117217670053	0.0961566642861047	0.1817200689217838
0.8987829398732849	0.2617122492347902	0.2864891350428321
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4038056161358461	0.5139722149068839	0.1242228097258102
0.2345741289133712	0.6827423696747115	0.2231191137138608
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3197989645235716	0.5974567637566799	0.1832613829025209
0.1513657146861466	0.7644340246808411	0.2852088504465110
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4042820397538551	0.7629216431704390	0.1239855408428364
0.2372267577136038	0.9318060393202685	0.2236611374548156
0.4867330000000010	0.6800539999999984	0.0814719999999980

0.3194975486290274 0.8474103878583672 0.1815725053672450
0.1340328606879869 0.5121456653165238 0.2826900163670610
0.3205450000000027 0.5965610000000012 0.0195900000000009
0.1552376053833698 0.7648528194088637 0.1238260416655703
0.4861186487387628 0.9287057712807361 0.2244942455632100
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0708743465917424 0.8490831945806787 0.1811113605559493
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1542035198252724 0.5130022955493311 0.1239114209801940
0.4820327671849624 0.6709234663072239 0.2295487404324568
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0693733144850192 0.5977489561151975 0.1802345748176365
0.4010081106425936 0.7672285897051534 0.2862854104947054
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9039478715896304 0.5140221225545366 0.1236877852833791
0.7411817261709172 0.6828184512418760 0.2231586485047532
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8210524602397673 0.5978083396115348 0.1801407643197982
0.6584345731010668 0.7675298143450864 0.2861606515044561
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9034258808446768 0.7648926162095270 0.1237947740747876
0.7353666091293279 0.9288338711332157 0.2244676924891911

0.986733000000010	0.680055000000030	0.081471999999980
0.8205536057810519	0.8475673545727810	0.1814859350091766
0.6705050286677352	0.5121312179129264	0.2827443249961445
0.820546000000002	0.596561000000012	0.019590000000009
0.6525244080971492	0.7630744542747308	0.1239692080005569
0.9878453074610816	0.9321877769985356	0.2236797041745925
0.736733000000010	0.680055000000030	0.081471999999980
0.5692317684957529	0.8457287035637939	0.1825551541786420
0.9033922663728228	0.5149757509198531	0.2846106836368118
0.820546000000002	0.846561000000012	0.019590000000009
0.6524018993815122	0.5130058768831804	0.1239523464658096
0.9901543033537250	0.6870249723887711	0.2221204322856062
0.736733000000010	0.930055000000030	0.081471999999980
0.5704965375567657	0.5975418742599674	0.1833175282816858
0.9047916701886327	0.7644922798752574	0.2850244298636744
0.4284327999437615	0.5596620918989005	0.4059670581779581
0.4168908488628579	0.5417991368084569	0.3374889587058154
0.4783120832677125	0.4793179532597934	0.3111918971915476
0.2937151929628194	0.4800981693111875	0.3112138909408674
0.3863408437364157	0.4826259237817143	0.3846397635427555
0.403638999999983	0.263308000000021	0.054287000000022
0.2384798290669922	0.4314031724502448	0.1541659443025217

0.0706768705891371 0.0978271096943482 0.2512317244525383
0.4036389999999983 0.0133080000000021 0.0542870000000022
0.2385131161465902 0.1844284581935116 0.1541644610989725
0.0602071776104105 0.3429261709943873 0.2505669514983008
0.1536389999999983 0.0133080000000021 0.0542870000000022
0.4867901146591255 0.1808146269781118 0.1528759738250498
0.3258263232097198 0.3594010435446364 0.2607628652164287
0.1536389999999983 0.2633080000000021 0.0542870000000022
0.4859418980167320 0.4316204372468505 0.1542179385151174
0.3194067194070855 0.0974863965055622 0.2510461547134372
0.9036389999999983 0.2633080000000021 0.0542870000000022
0.7366290192793590 0.4297416762911487 0.1522519151079832
0.5694072882591410 0.0954743236319383 0.2514240916424354
0.9036389999999983 0.0133080000000021 0.0542870000000022
0.7361242415899303 0.1792902899212352 0.1527259118143957
0.5749666291758279 0.3430443971864939 0.2505056286507357
0.6536389999999983 0.0133080000000021 0.0542870000000022
0.9869538445702336 0.1808143419059693 0.152839797977238
0.8196193517514738 0.3467895536539108 0.2510537272065088
0.6536389999999983 0.2633080000000021 0.0542870000000022
0.9861962830090555 0.4296159459673323 0.1523136968981432
0.8182615504212021 0.0956585337343931 0.2514319929798479

0.403638999999983 0.763308000000021 0.054287000000022
0.2379565491506961 0.9323575081712814 0.1526857624370580
0.0670344963728162 0.5999009729136925 0.2492714888235812
0.403638999999983 0.513308000000021 0.054287000000022
0.2374182548132857 0.6800080682551343 0.1527189381773641
0.0714281710727582 0.8503366891156674 0.2508486576093809
0.153638999999983 0.513308000000021 0.054287000000022
0.4866610225057525 0.6798493384836344 0.1539483593708325
0.3185262607648251 0.8484813359644755 0.2511685871568614
0.153638999999983 0.763308000000021 0.054287000000022
0.4866844674450687 0.9294393079242939 0.1530292510233457
0.3088842968732772 0.5966544873571051 0.2538883963696377
0.903638999999983 0.763308000000021 0.054287000000022
0.7360290697957266 0.9296321964877631 0.1529304152090274
0.5803954120066522 0.5965935747802030 0.2540341751569947
0.903638999999983 0.513308000000021 0.054287000000022
0.7357891560318423 0.6800884026674169 0.1526112414459608
0.5679062625510886 0.8437094985822510 0.2517957371448578
0.653638999999983 0.513308000000021 0.054287000000022
0.9876711003228273 0.6820277508345239 0.1519136142143412
0.8224447999046173 0.8486978962484452 0.2510468436536835
0.653638999999983 0.763308000000021 0.054287000000022

0.9876450115759677 0.9323978803052391 0.1526346473259131

0.8254811456534252 0.5998059132758637 0.2490997340642296

TiH_{1.97}-NO₃H

10.193035999999993 -5.9205420000000002 0.0221310000000000

0.0000000000000000 11.7965890000000009 -0.0158720000000000

0.0000000000000000 0.0000000000000000 27.290389999999986

H N O Ti

97 1 3 48

Selective dynamics

Direct

0.0705460000000002 0.3465610000000012 0.0195900000000009

0.4040002648477449 0.0136599894880987 0.1238037936495860

0.2328498515978581 0.1721154472753254 0.2224214025262316

0.4867330000000010 0.4300550000000030 0.0814719999999980

0.3197920677219699 0.0964089394532132 0.1812267266900626

0.1534383178925650 0.2634305566448277 0.2840945738090822

0.0705460000000002 0.0965599999999966 0.0195900000000009

0.4044694594085359 0.2646870445967539 0.1239254607779022

0.2374749132666145 0.4347563082523277 0.2261429883841522

0.4867330000000010 0.1800550000000030 0.0814719999999980

0.3196006524457222 0.3463866207039030 0.1796034826522316

0.1531292353869836 0.0138031866810145 0.2859555594319700
0.3205450000000027 0.096559999999966 0.0195900000000009
0.1542009530217967 0.2646717051698234 0.1239169257898979
0.4911154170124805 0.4356643699812293 0.2262406208662668
0.2367330000000010 0.1800539999999984 0.0814719999999980
0.0697955801626421 0.3475886146189979 0.1816786227833894
0.4038005727630570 0.0154677512663953 0.2856389224844769
0.3205450000000027 0.346559999999966 0.0195900000000009
0.1533585967015092 0.0125318995724096 0.1237563410736591
0.4860217829536698 0.1798225200608734 0.2236488931094896
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0695626010901740 0.0964901005556710 0.1812247859779168
0.4022665044253599 0.2632064687011393 0.2841768695412408
0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9035026252114542 0.0137110512218861 0.1237962264775020
0.7373321873001175 0.1816627631288680 0.2239601987525481
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8204529135301227 0.0980786569001510 0.1813836509105635
0.6538040325337265 0.2647351103456979 0.2861948265232306
0.5705460000000002 0.096559999999966 0.0195900000000009
0.9040214878575997 0.2641806841594760 0.1238078533766206
0.7379808231734906 0.4310927261301812 0.2240196487591585

0.986733000000010	0.180055000000030	0.081471999999980
0.8202358933628064	0.3477150570267515	0.1817063524386704
0.6553285120443882	0.0182777193073954	0.2852043487370367
0.820546000000002	0.096559999999966	0.019590000000009
0.6541003729343994	0.2643436220834330	0.1238127246942037
0.9861295677016385	0.4310570579186722	0.2240521893730969
0.736733000000010	0.180053999999984	0.081471999999980
0.5705206119613643	0.3476224929872494	0.1816328606877247
0.9039414782769484	0.0154424621996977	0.2854147134663931
0.820546000000002	0.346559999999966	0.019590000000009
0.6539756999587490	0.0141766931497586	0.1237641244249430
0.9873068778022660	0.1799769796468115	0.2236346005244749
0.736733000000010	0.430055000000030	0.081471999999980
0.5702950267079979	0.0980129851966111	0.1814535544710414
0.9029813438019625	0.2648193438192336	0.2862279909014050
0.070546000000002	0.846561000000012	0.019590000000009
0.4038027935340610	0.5137989738556227	0.1244112913092205
0.2402486354682354	0.6792955383325118	0.2266913403860037
0.486733000000010	0.930055000000030	0.081471999999980
0.3204121553476678	0.5966587932891922	0.1838663567969514
0.1538125697725819	0.7647828429559029	0.2854637789282443
0.070546000000002	0.596561000000012	0.019590000000009

0.4046203574160245	0.7629894441666555	0.1243996129182326
0.2353542177046059	0.9315351873248047	0.2233412283633872
0.486733000000010	0.680053999999984	0.081471999999980
0.3202265715167162	0.8474523379266767	0.1813752481598328
0.1370511576386603	0.5073850855530543	0.2864959533631116
0.320545000000027	0.596561000000012	0.019590000000009
0.1541750793948393	0.7624775587412362	0.1240702605222493
0.4868068799842836	0.9346430183687383	0.2233132805245891
0.236733000000010	0.680055000000030	0.081471999999980
0.0701241352144509	0.8472687296634431	0.1815245156678152
0.3943898336586916	0.4968398641954209	0.2744255035558881
0.320545000000027	0.846561000000012	0.019590000000009
0.1540025328663913	0.5140361488584614	0.1240601548625137
0.4864524928156460	0.6787419477689319	0.2312532857698490
0.236733000000010	0.930055000000030	0.081471999999980
0.0708340513174391	0.5975478185128805	0.1818011036297048
0.4119753147959165	0.7854865946031256	0.2836818138420094
0.570546000000002	0.846561000000012	0.019590000000009
0.9037824455046517	0.5135839487630258	0.1238310971256552
0.7319031368175607	0.6790369525057672	0.2267122230158359
0.986733000000010	0.930055000000030	0.081471999999980
0.8197032759216851	0.5977684100023057	0.1817638474741662

0.6673482104927919	0.7880199938382393	0.2836139896172558
0.5705460000000002	0.5965610000000012	0.0195900000000009
0.9025041412640507	0.7625452883072850	0.1240576524430041
0.7409867940020488	0.9347922547925969	0.2232244077305218
0.9867330000000010	0.6800550000000030	0.0814719999999980
0.8202228561717988	0.8475824292805242	0.1811524732222082
0.6628922954161639	0.5066283992266344	0.2866406487095768
0.8205460000000002	0.5965610000000012	0.0195900000000009
0.6522179300161344	0.7630182382801967	0.1243486475506640
0.9901536521025469	0.9317930088936628	0.2232363597074531
0.7367330000000010	0.6800550000000030	0.0814719999999980
0.5699104659748879	0.8472143359647557	0.1814106992732327
0.9036807343549723	0.5150024059693553	0.2851316283406817
0.8205460000000002	0.8465610000000012	0.0195900000000009
0.6540056036994867	0.5140593374389227	0.1241002090026660
0.9876506981766265	0.6819467021397899	0.2239424035381043
0.7367330000000010	0.9300550000000030	0.0814719999999980
0.5693572362889507	0.5967624851407640	0.1834411125785914
0.9031339229652007	0.7649632277139155	0.2852923775985973
0.4711505300784069	0.5768247401049107	0.4233959503479028
0.4537837157322161	0.6253999620420176	0.3589230164630991
0.5427957455828927	0.5975386419210775	0.3315659309099780

0.3447907069683707	0.5938619209864494	0.3319906274179166
0.4047757937515688	0.5298779233544502	0.3981834685882014
0.4036389999999983	0.2633080000000021	0.0542870000000022
0.2374217839726073	0.4324455317777688	0.1536079706502650
0.0695065500060619	0.0963537939804161	0.2510717924668392
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.2363595494164064	0.1791674211235545	0.1520633869109071
0.0671761727220453	0.3454259963826769	0.2508794912787319
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4871426975844630	0.1806005803700828	0.1525635575726745
0.3159840957375749	0.3384728695323854	0.2472076431910431
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.4882979183361985	0.4325169458048953	0.1536445798555368
0.3196531377577371	0.0961914383494296	0.2510752519326452
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7369901144816996	0.4310030477765524	0.1529435407231352
0.5710494520006919	0.1003819611592208	0.2512589187081667
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7371992865043520	0.1812884261518424	0.1526278500625418
0.5707314699091917	0.3454091393868117	0.2508183426047100
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9868667134712948	0.1806604184757296	0.1525777069635178

0.8198238099403908	0.3470823955180733	0.2514779417885402
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9872732759973443	0.4308258440211801	0.1528886360701415
0.8222683182662420	0.1007631910124049	0.2511705991552406
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2368744404726889	0.9298847033084036	0.1525442263719923
0.0699620458694284	0.5984457886427066	0.2509484983365116
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.2382709774817063	0.6797040874945758	0.1537306722101505
0.0706165628350617	0.8481101422633393	0.2513215793956131
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.4856743941408934	0.6779672123925462	0.1549993273653570
0.3194236658002899	0.8509800384217634	0.2503251583796598
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.4872683380831281	0.9306457851449310	0.1526793652760077
0.3194436393598512	0.5983980210503046	0.2628940747384699
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7365471890713432	0.9305306237947889	0.1526809765212965
0.5718487528870779	0.5988354992013126	0.2642537541973609
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7349997325785214	0.6799364036129398	0.1536303378633135
0.5741534358894208	0.8558763002437406	0.2497358769210399

0.653638999999983	0.513308000000021	0.054287000000022
0.9869107132543927	0.6801033624813976	0.1527664330526007
0.8246425019163780	0.8511787156118213	0.2499128287127241
0.653638999999983	0.763308000000021	0.054287000000022
0.9866130594451291	0.9300589028041014	0.1524422044651850
0.8212850286903223	0.5984102881306363	0.2508977142708473

TiH_{1.97}-Hv-NO₂

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H	N	O	Ti
95	1	2	48

Selective dynamics

Direct

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0.4041796110675064	0.0135400821291455	0.1238663004478107
0.2393465213478110	0.1856888426952980	0.2260418954182135
0.486733000000010	0.430055000000030	0.081471999999980
0.3195782186709782	0.0974783572474291	0.1817343413088109
0.1400641997964299	0.2536191351022765	0.2847089376643253
0.070546000000002	0.096559999999966	0.019590000000009

0.4039640519415544	0.2648844502503645	0.1241665713861386
0.2354441600872722	0.4283267526599488	0.2246934516904669
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3201924936578361	0.3482040749802483	0.1850212063922269
0.1526970061058001	0.0137854671569424	0.2859743152119872
0.3205450000000027	0.096559999999966	0.0195900000000009
0.1543194379092150	0.2647825827098840	0.1241131375972899
0.4853766047203194	0.4283282401917566	0.2247408999436074
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0691199097968827	0.3465602667182007	0.1814751590110955
0.4022274854564538	0.0131705285163552	0.2855455553693554
0.3205450000000027	0.346559999999966	0.0195900000000009
0.1545895144194694	0.0155148037591451	0.1240093588629244
0.4852104991403567	0.1776057883388699	0.2236666826492385
0.2367330000000010	0.4300550000000030	0.0814719999999980
0.0701995112716659	0.0974629786588043	0.1817454364378921
0.4045073683376131	0.2533990229292642	0.2847001747912350
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.9029808787988148	0.0135212651362652	0.1238345067311526
0.7363290460503761	0.1802209086588623	0.2241957434053219
0.9867330000000010	0.4300550000000030	0.0814719999999980
0.8195903100322687	0.0968000088146318	0.1817122552094581

0.6548020820421525	0.2627181337696481	0.2865477775433890
0.5705460000000002	0.0965599999999966	0.0195900000000009
0.9032852899859424	0.2629078904952611	0.1236905279994837
0.7389709125106542	0.4313914954495177	0.2229298522197296
0.9867330000000010	0.1800550000000030	0.0814719999999980
0.8196424683957566	0.3469310834936781	0.1811459186653511
0.6539129758776269	0.0166777567130973	0.2868811320822541
0.8205460000000002	0.0965599999999966	0.0195900000000009
0.6531332248729390	0.2629589877381405	0.1237130314923045
0.9849765756094135	0.4314498680427688	0.2228525923715643
0.7367330000000010	0.1800539999999984	0.0814719999999980
0.5698355070331219	0.3466540814193705	0.1815476219349305
0.9026902240153820	0.0133240858124222	0.2854413616210629
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6532997113766134	0.0131346448808936	0.1237968093842905
0.9848725482634172	0.1775544353716875	0.2236729243213982
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5694856798676253	0.0967306097813096	0.1816513421831443
0.8995817472655436	0.2629888443591976	0.2865730053257433
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4035965197004303	0.5136318131294583	0.1241827508640920
0.2381537264007575	0.6798098836655475	0.2241684469635379

0.486733000000010 0.930055000000030 0.081471999999980
0.3205824061965735 0.5969257872273029 0.1836505013219804
0.1521675748104642 0.7636176593418561 0.2850478961510040
0.070546000000002 0.596561000000012 0.019590000000009
0.4043498344916679 0.7631105334597001 0.1239319427410553
0.2357043989248679 0.9295144659270939 0.2233826838126506
0.486733000000010 0.680053999999984 0.081471999999980
0.3196189246023755 0.8467914087108928 0.1814967164005098
0.1361102645499813 0.5125449887306390 0.2815679696792512
0.320545000000027 0.596561000000012 0.019590000000009
0.1549035713782849 0.7637141501511753 0.1238344708397694
0.4859260297888759 0.9310564969075122 0.2240155649448710
0.236733000000010 0.680055000000030 0.081471999999980
0.0702320332499339 0.8479512073689980 0.1811648092034891
0.320545000000027 0.846561000000012 0.019590000000009
0.1544326288170349 0.5128937192036193 0.1239255141824135
0.4866473303158871 0.6806563720947567 0.2264371804968166
0.236733000000010 0.930055000000030 0.081471999999980
0.0699961370499846 0.5975861570037245 0.1801886440997251
0.4037888400565688 0.7711019725215411 0.2854185010608676
0.570546000000002 0.846561000000012 0.019590000000009
0.9034889709096511 0.5133801931744995 0.1237206217498265

0.7341733996961304 0.6796835085783482 0.2242553644513907
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8200177484269152 0.5976596662312513 0.1801567471918812
0.6589429815637365 0.7714317889894113 0.2853801308358616
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9024479073551352 0.7637341612908614 0.1237967283297990
0.7376934678620332 0.9311783177285541 0.2240661639595775
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8196365021553920 0.8469949998134285 0.1814791200472544
0.6681857015239189 0.5127415369282948 0.2815269549159428
0.8205460000000002 0.5965610000000012 0.0195900000000009
0.6524209005512440 0.7632598066324325 0.1239246336285117
0.9866482104455351 0.9297329030937350 0.2234606975383154
0.7367330000000010 0.6800550000000030 0.0814719999999980
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0.9039158905364898 0.5161143683245019 0.2839817956303429
0.8205460000000002 0.8465610000000012 0.0195900000000009
0.6520235686043883 0.5129641304077982 0.1239837785711746
0.9889833422827186 0.6849866550666244 0.2221971739123910
0.7367330000000010 0.9300550000000030 0.0814719999999980
0.5688319967083508 0.5970610979871287 0.1837186805990190
0.9028934332745111 0.7636233061413706 0.2849820407465413

0.4249044563039452 0.5572497749130879 0.3204243931307257
0.4758275740467045 0.4734093753990458 0.3101123795964061
0.2894371754819839 0.4740853665188641 0.3100427209551267
0.4036389999999983 0.2633080000000021 0.0542870000000022
0.2383988878853653 0.4310809486123098 0.1542276093830108
0.0682976565105994 0.0947977160495882 0.2510109678222360
0.4036389999999983 0.0133080000000021 0.0542870000000022
0.2377593304996604 0.1828151154885824 0.1537735866516492
0.0609285488757840 0.3430742466214043 0.2504275508893528
0.1536389999999983 0.0133080000000021 0.0542870000000022
0.4865323575952177 0.1805207852467607 0.1527928008204797
0.3203568686172041 0.3491020864856638 0.2584735527634943
0.1536389999999983 0.2633080000000021 0.0542870000000022
0.4855818582338716 0.4312212259406639 0.1543302080258320
0.3186311504586999 0.0943827923049100 0.2509978561123922
0.9036389999999983 0.2633080000000021 0.0542870000000022
0.7359175680159679 0.4296150359582962 0.1523754133927059
0.5694310036769682 0.0969781278398598 0.2515207882727612
0.9036389999999983 0.0133080000000021 0.0542870000000022
0.7363444641099475 0.1798332790377095 0.1526091740812529
0.5740750830559852 0.3429957306395985 0.2505387628584883
0.6536389999999983 0.0133080000000021 0.0542870000000022

0.9868072029811621	0.1804110493347416	0.1527533630846165
0.8198324965942776	0.3476298193676594	0.2510158061548193
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9866913733443506	0.4295727301406512	0.1523470466567188
0.8194281301697228	0.0971161259197471	0.2516213991327231
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2373927475279442	0.9311667476648557	0.1525664386349702
0.0679677683980243	0.5995782912741657	0.2490154810070581
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.2379819622188116	0.6796741898553929	0.1529525946484817
0.0702227168939830	0.8481661966916749	0.2509842689635886
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.4862720895714691	0.6794947092191453	0.1537873737248647
0.3188213571367041	0.8480552705742530	0.2509083542299789
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.4868513872953095	0.9296135822270458	0.1529921656320905
0.3185103729059596	0.5964132282309326	0.2555062862389126
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7358437951954321	0.9298023090776474	0.1529524903960224
0.5697662231504763	0.5965126421080278	0.2556386185643177
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7348316104471192	0.6799723283247333	0.1529455860346487

0.5725150959013606	0.8531673334081938	0.2516817315016349
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9870820385005988	0.6811797105416216	0.1519507120749231
0.8212368956124824	0.8480869426521226	0.2508558553541103
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9868353510317194	0.9311030517812895	0.1525211180493224
0.8239304463854972	0.5995110962849853	0.2489475308560553

TiH_{1.97}-NO₂

10.1930359999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H	N	O	Ti
96	1	2	48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4040375928205859	0.0139365369742579	0.1238243732273458
0.2331520524418375	0.1731710814946190	0.2227294533383707
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3198404004533534	0.0967515409199365	0.1813797079695842
0.1537282966541418	0.2634031248461804	0.2847385929512942

0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4044193049956004	0.2648295191243148	0.1239369249338438
0.2373832435020395	0.4338659043695081	0.2257325551932705
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3196623455416675	0.3467727021428509	0.1800495696334179
0.1529800082659898	0.0140261316563998	0.2859777380722753
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1541926623904171	0.2647822277250412	0.1239309171520491
0.4893281593839359	0.4337293561155635	0.2257614192784338
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0699344748660360	0.3477990825868219	0.1818861082058510
0.4037561541664175	0.0151884169355836	0.2857624361416944
0.3205450000000027	0.3465599999999966	0.0195900000000009
0.1533522348061903	0.0129450032868915	0.1237886157038014
0.4863002467287984	0.1804948874924825	0.2239850752098838
0.2367330000000010	0.4300550000000030	0.0814719999999980
0.0696037627026044	0.0966994513414298	0.1813772665749006
0.4015993480017148	0.2632951342841393	0.2847375471776238
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.9036934489432435	0.0139675959796586	0.1238127423238583
0.7373218816680951	0.1817418951544320	0.2241476490375670
0.9867330000000010	0.4300550000000030	0.0814719999999980

0.8204289859337206	0.0980941113719504	0.1815604551135233
0.6537725164758863	0.2647939511442852	0.2861890816937164
0.5705460000000002	0.0965599999999966	0.0195900000000009
0.9040654746551984	0.2642484855798267	0.1238453631528840
0.7373183185413613	0.4310555299539168	0.2242753894582841
0.9867330000000010	0.1800550000000030	0.0814719999999980
0.8201943458005772	0.3478165338906630	0.1817949615303402
0.6543530955220414	0.0168039073506700	0.2854521096497986
0.8205460000000002	0.0965599999999966	0.0195900000000009
0.6540335995025188	0.2643257504634335	0.1238461125617305
0.9865351513319918	0.4310478451843114	0.2242895371927378
0.7367330000000010	0.1800539999999984	0.0814719999999980
0.5704391009712196	0.3478278672636432	0.1818881803081705
0.9034459666173601	0.0151227234480800	0.2857156703200002
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6540888275455709	0.0143101885772400	0.1237856734129086
0.9871596893267027	0.1804811895586318	0.2240028470364707
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5703342144331195	0.0981467287836071	0.1815619644887214
0.9029807853699918	0.2648896413704329	0.2861502338276752
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4038773384574335	0.5141198324313934	0.1243977495852443

0.2393272670232140 0.6799174807157586 0.2260586295627273
0.4867330000000010 0.9300550000000030 0.0814719999999980
0.3203618779708253 0.5970921505271436 0.1835904447117164
0.1536834503576506 0.7649662992230142 0.2855160564257126
0.0705460000000002 0.5965610000000012 0.0195900000000009
0.4044869868060694 0.7633218030334150 0.1243468875864198
0.2354769491172672 0.9315802464100464 0.2235032912392146
0.4867330000000010 0.6800539999999984 0.0814719999999980
0.3204420721983789 0.8476708414933525 0.1813916348055671
0.1425683772965784 0.5099303323794399 0.2863437410977174
0.3205450000000027 0.5965610000000012 0.0195900000000009
0.1541150604818813 0.7628894667006790 0.1240307077572950
0.4870642254739587 0.9337370785245249 0.2236620372496554
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0700351489008395 0.8474075614462462 0.1815820166373036
0.3952538422513083 0.4986426359602595 0.2756062079128657
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1539045063790452 0.5141437064507806 0.1240317441679771
0.4860621804081662 0.6792694743100014 0.2289125110555409
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0705567951830574 0.5976483571259817 0.1818011885236186
0.4085406249741521 0.7799279406392386 0.2835077119975675

0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9037536166469210 0.5137790777748612 0.1238377130486948
0.7335102248930466 0.6797591026632787 0.2260323168272979
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8197188687274778 0.5977102976154522 0.1818433160044775
0.6631254824972291 0.7796782492382148 0.2834481372079260
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9025129757902428 0.7628465216230857 0.1240312622789213
0.7396568642316235 0.9336830634689511 0.2236681821800564
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8198436003675090 0.8475720175508942 0.1814120437098058
0.6591059563127973 0.5097814180519288 0.2864168764414604
0.8205460000000002 0.5965610000000012 0.0195900000000009
0.6525509708007157 0.7632596196684084 0.1243233816264187
0.9890906046496184 0.9314549567465225 0.2235339957900012
0.7367330000000010 0.6800550000000030 0.0814719999999980
0.5701086391796873 0.8475770660991871 0.1816472501878652
0.9035554150626771 0.5150114895513654 0.2853942064801255
0.8205460000000002 0.8465610000000012 0.0195900000000009
0.6539034383494720 0.5141155424906916 0.1240678570764408
0.9871656377387767 0.6815788904373530 0.2241124388768368
0.7367330000000010 0.9300550000000030 0.0814719999999980

0.5692432096547345	0.5971093648232483	0.1836205411419759
0.9033853216664185	0.7649459164935171	0.2855041309908336
0.4439399547224624	0.5958664166347789	0.3593697968809744
0.5374744796340967	0.5987982820881411	0.3343722943821779
0.3536675973414913	0.5990536156881463	0.3343368552361887
0.4036389999999983	0.2633080000000021	0.0542870000000022
0.2372859737997213	0.4323480994405134	0.1535085689008969
0.0691958187669628	0.0964119590521038	0.2512280234646103
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.2365170506388947	0.1797272363781897	0.1522094252546913
0.0685669441831680	0.3463080911836018	0.2512896422655702
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4871203767015732	0.1809499798145908	0.1526791204031802
0.3156873872820631	0.3391884487098390	0.2480032182905288
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.4881429299322437	0.4324134408407862	0.1535167392632280
0.3197389436296058	0.0964087717024883	0.2512643827948289
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7369397926041096	0.4310168897048908	0.1529806654578947
0.5706946870459693	0.0997563323546314	0.2513170266194611
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7372174112643549	0.1812691742841095	0.1527174247739028

0.5702099759721502	0.3462527910154812	0.2513301607980715
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9870677072108492	0.1809043368470641	0.1527072207967733
0.8198877069121701	0.3476100090980250	0.2514488199914082
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9871645145612286	0.4309347885343109	0.1529310123095142
0.8214798308710337	0.0997913557800281	0.2513073442261654
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2368596157960223	0.9302241118728620	0.1525938446876442
0.0700255022192598	0.5984686272663572	0.2510676567932846
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.2379272478356583	0.6800393428351477	0.1535755598985372
0.0703264547412610	0.8479779722001103	0.2513888285791752
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.4860751384613453	0.6790316920938121	0.1546786525068084
0.3194050300262141	0.8504293697101718	0.2504483168602681
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.4874034081429200	0.9309168109981393	0.1527388508631541
0.3201740781367462	0.5984907642833600	0.2596951441944544
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7367842565086338	0.9307983678586514	0.1527349667107015
0.5707193120763906	0.5983776097169307	0.2595599603288309

0.903638999999983	0.513308000000021	0.054287000000022
0.7352341879060076	0.6800239727710958	0.1535620072377499
0.5723864376855851	0.8524708859330455	0.2503889185837114
0.653638999999983	0.513308000000021	0.054287000000022
0.9868141821510248	0.6804142906094730	0.1527390598677413
0.8233029142504604	0.8501676394278653	0.2504542985955756
0.653638999999983	0.763308000000021	0.054287000000022
0.9864958382175768	0.9301823283522189	0.1525797440747518
0.8206167337225745	0.5982927113325145	0.2511670257850866

TiH_{1.97}-Hv-NO₂H

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H	N	O	Ti
96	1	2	48

Selective dynamics

Direct

0.070546000000002	0.346561000000012	0.019590000000009
0.4037597388245290	0.0136586035900759	0.1239001188003040
0.2385407121330142	0.1862819460942947	0.2260686800582234
0.486733000000010	0.430055000000030	0.081471999999980

0.3193340157726455	0.0978083673342992	0.1818896642270957
0.1403425518398625	0.2573060943856952	0.2843741765983693
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4033643933411434	0.2642633014943127	0.1241228160110828
0.2309674653518158	0.4274295782617226	0.2246528886399480
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3198355006030267	0.3491330112713584	0.1845698247906143
0.1521104075183139	0.0142124812300106	0.2858752458814285
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1535338224361888	0.2641373816154417	0.1240294549665721
0.4849414734608166	0.4275871297564993	0.2247730380893065
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0679491429821054	0.3461506518842564	0.1812938120481374
0.4014271743153326	0.0129889988298840	0.2856370064268134
0.3205450000000027	0.3465599999999966	0.0195900000000009
0.1544417597417121	0.0153314914913992	0.1240049811620785
0.4850635495621928	0.1778000318177047	0.2240895506049281
0.2367330000000010	0.4300550000000030	0.0814719999999980
0.0696982781911298	0.0975620375925541	0.1817606892838960
0.4029041231667350	0.2589127414256047	0.2847119963923908
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.9028557567111429	0.0132448843084791	0.1238442416729679

0.7347569479639851	0.1787400653548562	0.2240507928176369
0.986733000000010	0.430055000000030	0.081471999999980
0.8184059683193731	0.0956821597217632	0.1816162246314627
0.6529927846724223	0.2608672885741670	0.2866223266730401
0.570546000000002	0.096559999999966	0.019590000000009
0.9026328906504354	0.2628087842591770	0.1237408380380886
0.7376393428674423	0.4309517063219790	0.2236576203622660
0.986733000000010	0.180055000000030	0.081471999999980
0.8184680138581319	0.3461815493558387	0.1813529046810595
0.6505950826733252	0.0115014614307132	0.2863203581095404
0.820546000000002	0.096559999999966	0.019590000000009
0.6528292070721847	0.2629461480256060	0.1238115725430717
0.9829388866085401	0.4308927146847805	0.2232285082252369
0.736733000000010	0.180053999999984	0.081471999999980
0.5692464142898654	0.3465222309546946	0.1818915360520788
0.9014931262881846	0.0129821992060852	0.2856685987968018
0.820546000000002	0.346559999999966	0.019590000000009
0.6527232302264275	0.0125205282810189	0.1237779326470541
0.9825821229095980	0.1762133981300144	0.2235403341770098
0.736733000000010	0.430055000000030	0.081471999999980
0.5686576111810843	0.0959886267756166	0.1817655912479632
0.8966716966755305	0.2604154446875289	0.2865449412971438

0.0705460000000002 0.8465610000000012 0.0195900000000009
0.4031609287952708 0.5133659966578007 0.1240804090244017
0.2346327805531376 0.6804533032880196 0.2238473634575612
0.4867330000000010 0.9300550000000030 0.0814719999999980
0.3190962654174554 0.5967492315144100 0.1827440592218067
0.1511837521017094 0.7631914891086747 0.2858235000349144
0.0705460000000002 0.5965610000000012 0.0195900000000009
0.4033829706503740 0.7627098319779204 0.1239606447987321
0.2363816971682246 0.9301147814233719 0.2240154864601572
0.4867330000000010 0.6800539999999984 0.0814719999999980
0.3189684817040085 0.8466142687456779 0.1818538695315307
0.1403171640477244 0.5098195463716325 0.2846636529215424
0.3205450000000027 0.5965610000000012 0.0195900000000009
0.1541390831956670 0.7638634605179420 0.1239007518395313
0.4850108163924386 0.9288225203664253 0.2242011043838290
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0699138379244316 0.8474595605544564 0.1814775841524664
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1533992136523932 0.5127706396351480 0.1239235284667444
0.4828195808042980 0.6748122814466755 0.2271312435964092
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0689293876688683 0.5967595442701192 0.1812938190581780

0.4021257037514538	0.7648051150480117	0.2864089252087548
0.5705460000000002	0.8465610000000012	0.0195900000000009
0.9029126167832153	0.5134467991594168	0.1238263653170392
0.7394337619697953	0.6817739996267930	0.2233021328875381
0.9867330000000010	0.9300550000000030	0.0814719999999980
0.8199953814824638	0.5969774028332339	0.1811356922087659
0.6554563029529441	0.7665776518928271	0.2859772636308187
0.5705460000000002	0.5965610000000012	0.0195900000000009
0.9035437127442338	0.7639016280039369	0.1238084642463348
0.7351216764638098	0.9285097003514264	0.2241228762932252
0.9867330000000010	0.6800550000000030	0.0814719999999980
0.8199467606469432	0.8470368800052525	0.1815384900550285
0.6605639370195854	0.5140290056143064	0.2843770993108803
0.8205460000000002	0.5965610000000012	0.0195900000000009
0.6524709876316407	0.7626143266849836	0.1238920523552985
0.9864627337392521	0.9299366067713463	0.2237956471947181
0.7367330000000010	0.6800550000000030	0.0814719999999980
0.5687681947750858	0.8459863015567104	0.1820792127640166
0.9016095779447744	0.5130641950686053	0.2853452261561972
0.8205460000000002	0.8465610000000012	0.0195900000000009
0.6520669610613778	0.5128356233742698	0.1239577372442318
0.9876244234023620	0.6825376781091712	0.2233440245037825

0.736733000000010 0.930055000000030 0.081471999999980
0.5696726264268290 0.5971826467618601 0.1823307635016854
0.9033222481213382 0.7637559171223448 0.2855805761996585
0.4992982761405778 0.5192509510239603 0.3760279245730592
0.4470804333451892 0.4980447528611993 0.3086035096045467
0.3228021974096555 0.4849668223661435 0.3100703582929467
0.4682119051573015 0.4464663601736661 0.3526121230383941
0.403638999999983 0.263308000000021 0.054287000000022
0.2374101072668596 0.4305302431045040 0.1537175050385316
0.0679003213832878 0.0957685636081073 0.2510515719058243
0.403638999999983 0.013308000000021 0.054287000000022
0.2371745108010518 0.1825652026702938 0.1537618262316876
0.0574701631574409 0.3410773017116989 0.2502658158907602
0.153638999999983 0.013308000000021 0.054287000000022
0.4862067867671833 0.1805171902108794 0.1529561023662671
0.3202956388328578 0.3544823881714976 0.2574105818896047
0.153638999999983 0.263308000000021 0.054287000000022
0.4852133263582676 0.4306902512417650 0.1539143821864258
0.3180297354390182 0.0962119590629193 0.2511403065937986
0.903638999999983 0.263308000000021 0.054287000000022
0.7356567242068770 0.4296293939279376 0.1526501276727896
0.5684372642737611 0.0949494431221159 0.2514981018889718

0.903638999999983	0.013308000000021	0.054287000000022
0.7354273128363452	0.1790037914927496	0.1526436854109457
0.5724671358063934	0.3428922109743194	0.2511158127340880
0.653638999999983	0.013308000000021	0.054287000000022
0.9860829454591818	0.1800923937031561	0.1527200881743531
0.8177587840054285	0.3459244803032481	0.2512023969144927
0.653638999999983	0.263308000000021	0.054287000000022
0.9855143986316717	0.4295798211387888	0.1524891789984507
0.8165287557626829	0.0945624012474386	0.2513917449790349
0.403638999999983	0.763308000000021	0.054287000000022
0.2370452916767959	0.9310273204631901	0.1528000426214761
0.0673785953842595	0.5971889579738632	0.2507741039795010
0.403638999999983	0.513308000000021	0.054287000000022
0.2364206272015222	0.6795503672410579	0.1528861332970101
0.0699567138325721	0.8477697084706859	0.2511580323473696
0.153638999999983	0.513308000000021	0.054287000000022
0.4859327445761991	0.6793807210952721	0.1535715749630254
0.3183908348210953	0.8466646633637802	0.2516054815758115
0.153638999999983	0.763308000000021	0.054287000000022
0.4860127350361935	0.9294677837093547	0.1529022130435974
0.3130187740377300	0.5960473978235998	0.2531043624203397
0.903638999999983	0.763308000000021	0.054287000000022

0.7356360851965303	0.9293444318218188	0.1527759597198973
0.5758736862388628	0.5986231798457052	0.2528293999146513
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7364308030805159	0.6800514508626367	0.1526432063963033
0.5681500493292581	0.8458001560898608	0.2513535466269745
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9868088460639203	0.6805760165366388	0.1524850489673726
0.8207615511513334	0.8477106957119165	0.2512583289321514
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9868785703991659	0.9309366474247799	0.1526449997702121
0.8218780604986480	0.5981103810534666	0.2505523640877635

TiH_{1.97}-NO₂H

10.1930359999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H	N	O	Ti
97	1	2	48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4034116187741696	0.0121858305093388	0.1238800950955526

0.2297405923355474 0.1671659344869532 0.2217795566339802
0.4867330000000010 0.4300550000000030 0.0814719999999980
0.3181453021655520 0.0941903833698089 0.1808478807445770
0.1516999669305192 0.2592028282261638 0.2845519628024782
0.0705460000000002 0.0965599999999966 0.0195900000000009
0.4035655997135870 0.2629621587476149 0.1238008548593196
0.2385698160707800 0.4321097582301884 0.2260692806266780
0.4867330000000010 0.1800550000000030 0.0814719999999980
0.3176958906157427 0.3438838511633032 0.1793409914683426
0.1503651662805092 0.0098095332661501 0.2854362344288184
0.3205450000000027 0.0965599999999966 0.0195900000000009
0.1526114932597645 0.2627815841945434 0.1238800339008864
0.4856129224156747 0.4288176645462558 0.2244793206807293
0.2367330000000010 0.1800539999999984 0.0814719999999980
0.0685385255415164 0.3454563421458841 0.1817673183638911
0.4001018652601102 0.0104570221028516 0.2851209930909571
0.3205450000000027 0.3465599999999966 0.0195900000000009
0.1519509070324652 0.0109497456697423 0.1236346670922122
0.4841984819411842 0.1781019069180160 0.2238868989112377
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0680392157553640 0.0940939578419080 0.1808539823507972
0.3980539428488348 0.2579877461912483 0.2846478552903645

0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9016400244725612 0.0118205532843098 0.1238864794972983
0.7352954362194957 0.1791346844074450 0.2242833086259479
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8184471074823199 0.0956930179081746 0.1816268055180458
0.6507911525617828 0.2614321170956956 0.2862259323608007
0.5705460000000002 0.0965599999999966 0.0195900000000009
0.9027020189727819 0.2625608477048176 0.1238418330774833
0.7342491480337098 0.4276261621086194 0.2246827186214074
0.9867330000000010 0.1800550000000030 0.0814719999999980
0.8184469861476631 0.3457402315778909 0.1821119279397404
0.6558070691730770 0.0214525920731661 0.2858375386172088
0.8205460000000002 0.0965599999999966 0.0195900000000009
0.6530539659602438 0.2627102119069992 0.1238433248834494
0.9848667695524305 0.4275756199536556 0.2245475294470773
0.7367330000000010 0.1800539999999984 0.0814719999999980
0.5684621787878255 0.3455444732398962 0.1819712519298224
0.9011149238891168 0.0106910941667636 0.2850208961339193
0.8205460000000002 0.3465599999999966 0.0195900000000009
0.6529394591383777 0.0128221166346104 0.1239361655761094
0.9854285845537161 0.1774403784454696 0.2237250326252202
0.7367330000000010 0.4300550000000030 0.0814719999999980

0.5690058669674021	0.0957987847567345	0.1817132823584551
0.9019417072109511	0.2615428740266278	0.2855387320494424
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4030239119002634	0.5133320799529830	0.1244468594044617
0.2383166867635340	0.6745311725831454	0.2264258963328869
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3175572845768007	0.5945774854323078	0.1826380577518773
0.1518959243732256	0.7621220238473686	0.2851742235153223
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4028864865732986	0.7617651688995658	0.1244253348118068
0.2310690448376901	0.9294393756071356	0.2223341428628669
0.4867330000000010	0.6800539999999984	0.0814719999999980
0.3185851277026752	0.8449962184250581	0.1803371970532962
0.1437359833681048	0.5067685859150886	0.2856534309265956
0.3205450000000027	0.5965610000000012	0.0195900000000009
0.1519836207300255	0.7605451457075185	0.1239876051452614
0.4863849915904228	0.9283348488961418	0.2250235564117369
0.2367330000000010	0.6800550000000030	0.0814719999999980
0.0682873322085579	0.8447074558321584	0.1811185098001982
0.3966078646118664	0.4799446179128530	0.2802794670917298
0.3205450000000027	0.8465610000000012	0.0195900000000009
0.1520634016170763	0.5118856460820773	0.1240074192396728

0.4823585529168249 0.6790530028932058 0.2248313555191876
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0684995269179762 0.5948941644459160 0.1820274770332488
0.3941427193068273 0.7759771806124699 0.2811779865288704
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9020591113942895 0.5114371664175156 0.1238860637079610
0.7312739919644088 0.6754645553460433 0.2252774332836245
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8175861452005543 0.5949394785249020 0.1822051581663405
0.6696235969837357 0.7658435336577119 0.2788850664984596
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9009721971930542 0.7603756350890428 0.1239100991178071
0.7342174425260033 0.9277250058036739 0.2253338456324516
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8183024391347553 0.8451751400898490 0.1804433818268234
0.6512009031754323 0.5091090037770754 0.2865965551830955
0.8205460000000002 0.5965610000000012 0.0195900000000009
0.6511397901552427 0.7615407075977940 0.1245095531548717
0.9905091793080680 0.9294637364411875 0.2224857432245574
0.7367330000000010 0.6800550000000030 0.0814719999999980
0.5689596026273285 0.8463017196482483 0.1830690603309073
0.9014580504748114 0.5117951498098443 0.2858988627871400

0.8205460000000002	0.8465610000000012	0.0195900000000009
0.6525901770537608	0.5121636764660161	0.1239999606628866
0.9834315818500022	0.6765264267789770	0.2243139766753600
0.7367330000000010	0.9300550000000030	0.0814719999999980
0.5673790154677619	0.5948938354484522	0.1836313767403561
0.9014857855616173	0.7619464411839079	0.2853744898621445
0.4889825676246000	0.8084600784497622	0.3515806676395937
0.4802946260660063	0.6515932833470228	0.3180218671811222
0.5585382028087803	0.8011887530399698	0.3344007568496933
0.3597368960906950	0.6008390219098196	0.3347561052190077
0.4036389999999983	0.2633080000000021	0.0542870000000022
0.2355027608579414	0.4300945931903047	0.1532897410091335
0.0670479125038541	0.0928276993009633	0.2507184231872941
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.2351892890959263	0.1774138236846424	0.1517716578775513
0.0680377522204737	0.3429976885731268	0.2510087168314697
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4861275257609328	0.1790683571245959	0.1526854570730526
0.3124814575072189	0.3322140598603461	0.2470112793778367
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.4863580872457550	0.4300837680398591	0.1531311352527681
0.3172526570619585	0.0925906830834173	0.2507782702239242

0.903638999999983	0.263308000000021	0.054287000000022
0.7352265515283061	0.4288905473507085	0.1531468642630515
0.5677376024461656	0.0968581195932864	0.2511519077831684
0.903638999999983	0.013308000000021	0.054287000000022
0.7359540408540153	0.1795454480048881	0.1529053788489882
0.5671048709937206	0.3432031579376795	0.2516628066005511
0.653638999999983	0.013308000000021	0.054287000000022
0.9853386833340184	0.1785994608426343	0.1525615526936892
0.8179715257620206	0.3451328039659392	0.2517591416233992
0.653638999999983	0.263308000000021	0.054287000000022
0.9853988482975190	0.4287009001874873	0.1531072891826072
0.8199242603968160	0.0963957930833527	0.2509393874921276
0.403638999999983	0.763308000000021	0.054287000000022
0.2353015738739074	0.9279253463832265	0.1521103048070490
0.0674953845605351	0.5949404254647019	0.2513100891724034
0.403638999999983	0.513308000000021	0.054287000000022
0.2355698535889789	0.6772135517612088	0.1534925834947319
0.0676057154806409	0.8434263473297691	0.2510587659314680
0.153638999999983	0.513308000000021	0.054287000000022
0.4846527646334121	0.6786892858483176	0.1551678459147462
0.3142346127093841	0.8478694056392453	0.2484523592512467
0.153638999999983	0.763308000000021	0.054287000000022

0.4867326466784468	0.9287461975967330	0.1531991946780830
0.3234997098938726	0.5953756226741752	0.2622221128195582
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7343034037004540	0.9286414254682408	0.1532208954196586
0.5638617526109438	0.5943425206537064	0.2563172451401270
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7336762480974705	0.6776639900345133	0.1534805568031634
0.5700676104522822	0.8489768704125628	0.2569313206361004
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9846920350917961	0.6776717283977963	0.1528863757807195
0.8252724678164041	0.8473703596594783	0.2486903921400112
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9848736683435814	0.9276912970305147	0.1521393742791514
0.8174763591129540	0.5943381610351703	0.2517750038810963

TiH_{1.97}-Hv-NO

10.1930359999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H	N	O	Ti
95	1	1	48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4043087867598946	0.0137693130340386	0.1239719830196328
0.2391012640188870	0.1831232838169554	0.2253363672401549
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3203922663759633	0.0979611816838903	0.1824450607547702
0.1424157754387188	0.2537697494862755	0.2836839046272168
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4037698495296131	0.2638078979902668	0.1240797561451428
0.2338567365824661	0.4288604463004916	0.2246336159472060
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3191395226791333	0.3475685795097181	0.1832834450951613
0.1535750218016035	0.0142557296243862	0.2859879697842941
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1538437392880004	0.2638969416083483	0.1240253183761947
0.4859443704222188	0.4273526852619186	0.2239380333125723
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0689288151442335	0.3464949629711200	0.1816761548972363
0.4037658329031664	0.0139751208186722	0.2860862201475828
0.3205450000000027	0.3465599999999966	0.0195900000000009
0.1552982540832713	0.0145554090163504	0.1239937953119376
0.4867626397716262	0.1793879047577392	0.2243812205069985

0.236733000000010 0.430055000000030 0.081471999999980
0.0701013829756244 0.0971263845307795 0.1813038691679239
0.4064512164763195 0.2641665499136724 0.2866989239055145
0.570546000000002 0.346561000000012 0.019590000000009
0.9037279234335094 0.0133099474187475 0.1238260814826372
0.7370052694668877 0.1806276064749900 0.2244499647457981
0.986733000000010 0.430055000000030 0.081471999999980
0.8197307550391084 0.0968642225091215 0.1816665677480441
0.6544284569201291 0.2633266426525579 0.2864542781096218
0.570546000000002 0.096559999999966 0.019590000000009
0.9033415032530651 0.2633257574984305 0.1237482273205558
0.7390465414678571 0.4317890823426402 0.2239494988232867
0.986733000000010 0.180055000000030 0.081471999999980
0.8197725072900883 0.3471001687681811 0.1816935589967557
0.6542524077872479 0.0157323282785439 0.2864751447694832
0.820546000000002 0.096559999999966 0.019590000000009
0.6534522599938910 0.2635083514894911 0.1239041606116822
0.9856259626812656 0.4315363421210750 0.2235887917820346
0.736733000000010 0.180053999999984 0.081471999999980
0.5701133465005682 0.3470097631399881 0.1817347582677928
0.9039372426838526 0.0140472196178042 0.2854004041598479
0.820546000000002 0.346559999999966 0.019590000000009

0.6534953119725678	0.0133757670798489	0.1238939700285215
0.9855854491916609	0.1780754116980410	0.2236324665941923
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5697947261048162	0.0969617667992856	0.1818835039036151
0.9000753533358020	0.2623921848373341	0.2869240012575728
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4034257661291945	0.5133312832319414	0.1240342166887066
0.2389608148364114	0.6795612785996301	0.2252932330616237
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3193353416457836	0.5956238574457678	0.1832917980161965
0.1535858873694604	0.7638604447072371	0.2860797354900459
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4038364013849426	0.7632268132653846	0.1240362520760558
0.2397555149456751	0.9318594876111993	0.2247677448651746
0.4867330000000010	0.6800539999999984	0.0814719999999980
0.3204264309909868	0.8465039736081517	0.1824108064174413
0.1426246155858080	0.5134754805013648	0.2837941055521885
0.3205450000000027	0.5965610000000012	0.0195900000000009
0.1553412374468273	0.7638243163592294	0.1240351120684154
0.4865994760590341	0.9313993377242203	0.2243233446824937
0.2367330000000010	0.6800550000000030	0.0814719999999980
0.0713767466499018	0.8476262210275356	0.1816510017856958

0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1539136885821308 0.5131648490032857 0.1240472668631570
0.4859546568710980 0.6827245266441330 0.2239205687347419
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0702678268585057 0.5970446623383133 0.1813391786661356
0.4064093716904644 0.7669338604683409 0.2866135900244613
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9037013446491318 0.5135893626623195 0.1238538036103745
0.7410244218685486 0.6824321181002283 0.2236275861470458
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8212112492342428 0.5977402078916793 0.1813313699544441
0.6588585212382558 0.7686585293709585 0.2840768473735117
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9047527140620963 0.7639034615572552 0.1238116966437999
0.7390596908711168 0.9313562967432710 0.2238877085268607
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8211679762475755 0.8475833480278866 0.1812822517864913
0.6588773824230856 0.5154152426213593 0.2840862783779737
0.8205460000000002 0.5965610000000012 0.0195900000000009
0.6531261181656502 0.7631558440676939 0.1239036537298049
0.9884446865676427 0.9291139826010273 0.2234563625756949
0.7367330000000010 0.6800550000000030 0.0814719999999980

0.5701429877766885 0.8472418146511158 0.1816851474539421
0.9040685953661683 0.5147012856848742 0.2855242995330473
0.8205460000000002 0.8465610000000012 0.0195900000000009
0.6529367239739864 0.5131610911328724 0.1239378949714201
0.9883963238757766 0.6830622919086548 0.2234482759535223
0.7367330000000010 0.9300550000000030 0.0814719999999980
0.5708931085919670 0.5975959965154415 0.1806555817129900
0.9057932749869849 0.7653477266892696 0.2854308963682343
0.4307314190297372 0.5276933114089324 0.2948038001777995
0.3082765940850151 0.4661753949127725 0.3130456584208515
0.4036389999999983 0.2633080000000021 0.0542870000000022
0.2375022312528500 0.4305405724164862 0.1536423235879317
0.0690637311525711 0.0946641090629566 0.2504767198022139
0.4036389999999983 0.0133080000000021 0.0542870000000022
0.2374199014128817 0.1816447656779168 0.1534144419170735
0.0620063976840872 0.3432923643606482 0.2510189507312073
0.1536389999999983 0.0133080000000021 0.0542870000000022
0.4867340633152282 0.1805512479475457 0.1530460714401246
0.3184274537612806 0.3491574119802378 0.2550226152258511
0.1536389999999983 0.2633080000000021 0.0542870000000022
0.4855880166987888 0.4303998106563136 0.1536339511434154
0.3209992792238525 0.0986576355388946 0.2522113019967597

0.903638999999983	0.263308000000021	0.054287000000022
0.7366977113229887	0.4303138361203336	0.1528256769301135
0.5702901464883184	0.0972593303945853	0.2516956119717290
0.903638999999983	0.013308000000021	0.054287000000022
0.7367490803279289	0.1803078545118666	0.1527149682542626
0.5731418174870302	0.3452868714959719	0.2509539611788584
0.653638999999983	0.013308000000021	0.054287000000022
0.9863397264926762	0.1802244469477625	0.1526601656859618
0.8204873004765528	0.3477592275401115	0.2515243575100878
0.653638999999983	0.263308000000021	0.054287000000022
0.9863502402167476	0.4297838509836824	0.1526919978925474
0.8202858646724750	0.0971281419500249	0.2514771424969316
0.403638999999983	0.763308000000021	0.054287000000022
0.2382923884873857	0.9309266358039565	0.1531643560166107
0.0689754010974936	0.5986191479600038	0.2505449347770586
0.403638999999983	0.513308000000021	0.054287000000022
0.2377175385884237	0.6794272784284743	0.1534580718260360
0.0723396182587240	0.8481446037139214	0.2513092089669458
0.153638999999983	0.513308000000021	0.054287000000022
0.4857749341703130	0.6791057249784703	0.1535098452909803
0.3207156979935161	0.8463838742917462	0.2521709770021971
0.153638999999983	0.763308000000021	0.054287000000022

0.4867432998149682	0.9298833712962237	0.1530262848654534
0.3183750255096538	0.5933835530857682	0.2550073888315571
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7367313162163189	0.9301611048275419	0.1528018628101927
0.5724805939200466	0.5985925719405264	0.2516845819540792
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7379627873932694	0.6808236072684456	0.1525262792137620
0.5730555524578174	0.8523840154350528	0.2508752131538207
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9879682379937665	0.6807406503775268	0.1525571392893790
0.8232117722599382	0.8485542741971193	0.2508634439845215
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9879782425730429	0.9306764735855689	0.1525173316242619
0.8233967828676093	0.5992170835338247	0.2509171416312991

TiH_{1.97}-NO

10.1930359999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H	N	O	Ti
96	1	1	48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4048434659057626	0.0136056003300630	0.1238296846067506
0.2336875054046363	0.1729377595016023	0.2221831286406834
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3201712707530135	0.0968293323248574	0.1809345995511903
0.1545256003325863	0.2628737140262077	0.2848181141225083
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4049190738346853	0.2641146601358436	0.1238382139948140
0.2405726902381441	0.4356198744119958	0.2264294310272005
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3193123929851263	0.3465973595326494	0.1799327759981702
0.1537532299798687	0.0137537199650382	0.2854695800139573
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1532428609111224	0.2634405586707611	0.1238648334325429
0.4900753418228444	0.4344464316432743	0.2247813316824210
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0695240845791199	0.3467111161817793	0.1820406872163955
0.4019581878969904	0.0133391144231575	0.2844655999054787
0.3205450000000027	0.3465599999999966	0.0195900000000009
0.1537771090682518	0.0132678133192896	0.1235909239332616
0.4880471055922470	0.1807223357259804	0.2243204047419686

0.236733000000010	0.430055000000030	0.081471999999980
0.0701911303303801	0.0966236368506485	0.1809631894780725
0.4016350370257138	0.2620254486417059	0.2845281270774385
0.570546000000002	0.346561000000012	0.019590000000009
0.9024620300407592	0.0129708047559020	0.1238252231352795
0.7377343018121389	0.1798650379961315	0.2247647232355433
0.986733000000010	0.430055000000030	0.081471999999980
0.8196058573685270	0.0962862760948488	0.1820628027482915
0.6533010435661907	0.2633109155356712	0.2861208544739135
0.570546000000002	0.096559999999966	0.019590000000009
0.9031191688048515	0.2632182678089618	0.1238886750029755
0.7375768856737622	0.4307834564195005	0.2248047327560384
0.986733000000010	0.180055000000030	0.081471999999980
0.8194664434520739	0.3464829481695931	0.1821986196137784
0.6557819258537194	0.0160585420145212	0.2862223332727086
0.820546000000002	0.096559999999966	0.019590000000009
0.6545483048092884	0.2636852176701890	0.1239945604379809
0.9867780039397686	0.4298457736216698	0.2245491026570986
0.736733000000010	0.180053999999984	0.081471999999980
0.5701221320699078	0.3475004303202404	0.1821480186256784
0.9045170432148077	0.0123906856858013	0.2851911926397581
0.820546000000002	0.346559999999966	0.019590000000009

0.6537188301018669	0.0133437402340929	0.1239420332743547
0.9871388060027825	0.1798083906924732	0.2238873844024696
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5702969676579694	0.0963620684109318	0.1819682792864784
0.9035551307337456	0.2630792147819086	0.2860059237586360
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4033857718252102	0.5136729876898716	0.1242982428666329
0.2406363737314616	0.6779894349655605	0.2264559246904927
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3175230888153696	0.5954792300701710	0.1816979773736186
0.1548444870567051	0.7650896343703214	0.2848131584914577
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4034172393832471	0.7626385944570977	0.1242487856787675
0.2334673378825900	0.9336189963323830	0.2221018267482253
0.4867330000000010	0.6800539999999984	0.0814719999999980
0.3195070037708465	0.8463735637140302	0.1798404001234629
0.1438956454755958	0.5088573440298032	0.2865836329526834
0.3205450000000027	0.5965610000000012	0.0195900000000009
0.1532198943153067	0.7624851352320957	0.1239084505251087
0.4900042856201625	0.9287934443607770	0.2245827190170650
0.2367330000000010	0.6800550000000030	0.0814719999999980
0.0701714995530162	0.8469158583241497	0.1810785041061278

0.4047537942126017	0.4800565017200623	0.2849093089200426
0.3205450000000027	0.8465610000000012	0.0195900000000009
0.1524477295668066	0.5125898285529737	0.1239025429473619
0.4807738844249506	0.6769981073150507	0.2221416928607366
0.2367330000000010	0.9300550000000030	0.0814719999999980
0.0694934763475523	0.5962059321154565	0.1819451245762738
0.4047659712792781	0.7986828801876942	0.2847332037230481
0.5705460000000002	0.8465610000000012	0.0195900000000009
0.9030422852609954	0.5126086444519105	0.1239282921997308
0.7344935894433428	0.6789438037116945	0.2252466162207915
0.9867330000000010	0.9300550000000030	0.0814719999999980
0.8194655504380520	0.5968084282256100	0.1821261440671179
0.6821853143221044	0.7779495399700923	0.2820735552173426
0.5705460000000002	0.5965610000000012	0.0195900000000009
0.9022767212713613	0.7620527714700094	0.1238675330872842
0.7346250012708411	0.9283217546578455	0.2251213703580012
0.9867330000000010	0.6800550000000030	0.0814719999999980
0.8205216563725874	0.8470076283269182	0.1798713052314674
0.6557519097862337	0.5137148079989973	0.2864391902184630
0.8205460000000002	0.5965610000000012	0.0195900000000009
0.6520538252037255	0.7624630963230532	0.1244648038347574
0.9953016484181278	0.9338351696328193	0.2221132402446226

0.736733000000010	0.680055000000030	0.081471999999980
0.5692675368221685	0.8459153900127940	0.1834137750607591
0.9037708599682325	0.5140938766109803	0.2860173805765278
0.820546000000002	0.846561000000012	0.019590000000009
0.6535046861443465	0.5131178057031176	0.1240408146040250
0.9870533517111474	0.6803493598262416	0.2238821087851401
0.736733000000010	0.930055000000030	0.081471999999980
0.5690259227731128	0.5969799270007790	0.1834783490115232
0.9044547814240983	0.7655282719100307	0.2853410607257588
0.4896884890991208	0.6821554939704864	0.3044872514057680
0.3735401450049354	0.6239739123121476	0.3303009788986540
0.403638999999983	0.263308000000021	0.054287000000022
0.2357291799558143	0.4306366002180935	0.1531522167846018
0.0703178560797749	0.0965898518264967	0.2508601205059964
0.403638999999983	0.013308000000021	0.054287000000022
0.2370101098410231	0.1797802014977037	0.1519949935631955
0.0691740687581446	0.3450669180024361	0.2514322069210579
0.153638999999983	0.013308000000021	0.054287000000022
0.4879534603471601	0.1805424838264760	0.1528452325975579
0.3170690958024059	0.3387664815160338	0.2478114250980495
0.153638999999983	0.263308000000021	0.054287000000022
0.4872659477395413	0.4312496722610579	0.1532926171817616

0.3200871208438011	0.0965305508458083	0.2507545494601951
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7365063800640114	0.4303960774833898	0.1533023523184074
0.5707542980385336	0.0976258447054035	0.2514156117566716
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7366934816251099	0.1794070762433276	0.1532230998942289
0.5707719908994707	0.3467081268856498	0.2517291497059182
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9862156943335735	0.1798686805875716	0.1526422590812509
0.8202900414203019	0.3468645875343417	0.2518582863755569
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9862054146614307	0.4295834034430437	0.1531512637859169
0.8220196381378441	0.0970453641797655	0.2514843385433573
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2368946029432183	0.9302701168824092	0.1520013065450191
0.0689359163067191	0.5974139848167693	0.2512647754853893
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.2358842941362395	0.6781856923232735	0.1531168732944309
0.0705023573150125	0.8467918073274681	0.2510957364483895
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.4851457722544659	0.6793215554945260	0.1549208005852303
0.3170924103422236	0.8519250628334337	0.2477149187721456

0.153638999999983	0.763308000000021	0.054287000000022
0.4875997849752345	0.9294475834665289	0.1531320386147378
0.3238963777453138	0.5985879247440421	0.2625583825803572
0.903638999999983	0.763308000000021	0.054287000000022
0.7350448969368654	0.9294024023150124	0.1533377900478633
0.5665127942622252	0.6009984680030834	0.2579079007306226
0.903638999999983	0.513308000000021	0.054287000000022
0.7348706172946169	0.6788842711178820	0.1533935069427255
0.5665023860917923	0.8391862254694422	0.2578740624562030
0.653638999999983	0.513308000000021	0.054287000000022
0.9862100840187032	0.6794804061754771	0.1527367244286910
0.8296830554049707	0.8513687873466218	0.2477691504072868
0.653638999999983	0.763308000000021	0.054287000000022
0.9870994753373284	0.9300027748941136	0.1519715794364002
0.8221780652446696	0.5981872423233309	0.2516134795477861

TiH_{1.97}-Hv-NOH

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H N O Ti

96 1 1 48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4040159017892826	0.0137019036147253	0.1239297497447246
0.2394978022062661	0.1850131449810806	0.2255902218647856
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3199670489906072	0.0976807170721710	0.1823802316187273
0.1393284083015619	0.2527082327282174	0.2834249543528614
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4037210578830827	0.2636893230424804	0.1239340458234670
0.2356192032544412	0.4298739943256440	0.2241269856611166
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3205996558823442	0.3481704215841912	0.1839219716097472
0.1528483120975659	0.0141853171023140	0.2859866197517739
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1544447642193524	0.2645974304371644	0.1240108244913953
0.4864662085123658	0.4284239488355469	0.2245472500443306
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0694833173563367	0.3468375749256928	0.1810556554216561
0.4034139784577265	0.0141521735992444	0.2860972035832111
0.3205450000000027	0.3465599999999966	0.0195900000000009
0.1551663703319826	0.0149179084398431	0.1239832402423788

0.4863881238445935 0.1795425690452019 0.2243610133427545
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0702512485327355 0.0972559672458506 0.1812440994147489
0.4068562115154574 0.2629006191996032 0.2870606098391890
0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9035200831223648 0.0134140133485279 0.1238174165139950
0.7364538014501510 0.1805099183465744 0.2240540251454415
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8196162238325506 0.0968778603794255 0.1813761432295632
0.6547206352846848 0.2633224507410298 0.2867532242042954
0.5705460000000002 0.0965599999999966 0.0195900000000009
0.9032851194119961 0.2634004120763055 0.1237115065871249
0.7386996048707319 0.4320392839563920 0.2237158555530264
0.9867330000000010 0.1800550000000030 0.0814719999999980
0.8197152561127413 0.3471456584845469 0.1813572866300394
0.6543699681754092 0.0161050014528439 0.2868082461538890
0.8205460000000002 0.0965599999999966 0.0195900000000009
0.6530727227347392 0.2633925837070609 0.1238247340811528
0.9852108315955457 0.4320888264282210 0.2232169842267134
0.7367330000000010 0.1800539999999984 0.0814719999999980
0.5699025315478523 0.3468240916411200 0.1817943005265218
0.9033518286931314 0.0139160138853054 0.2852168860583595

0.8205460000000002 0.3465599999999966 0.0195900000000009
0.6531266434575536 0.0132351802797727 0.1238080167354033
0.9848889832435143 0.1773226194375316 0.2232203448335459
0.7367330000000010 0.4300550000000030 0.0814719999999980
0.5696060837867041 0.0969934279322398 0.1819096379604578
0.9000078374452970 0.2627088540991110 0.2862584866239572
0.0705460000000002 0.8465610000000012 0.0195900000000009
0.4037764129336194 0.5135770446339945 0.1239338329909677
0.2396463637789397 0.6785297189466204 0.2256881960175635
0.4867330000000010 0.9300550000000030 0.0814719999999980
0.3207865323524293 0.5966179479193808 0.1841290796170479
0.1528864160394963 0.7639382708640140 0.2860560476603937
0.0705460000000002 0.5965610000000012 0.0195900000000009
0.4037215423335009 0.7634749588715258 0.1239113362149608
0.2384960971012309 0.9314635352810193 0.2243987211750369
0.4867330000000010 0.6800539999999984 0.0814719999999980
0.3200266239291842 0.8465777373270693 0.1823774733652528
0.1399436648817254 0.5118479572835410 0.2835060964604685
0.3205450000000027 0.5965610000000012 0.0195900000000009
0.1552526253394947 0.7634876207647814 0.1240184236036615
0.4862281092187412 0.9311932887736309 0.2242869524347452
0.2367330000000010 0.6800550000000030 0.0814719999999980

0.0707536178725826 0.8474768453876237 0.1815181026638068
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1544989260599572 0.5133213573214629 0.1240127510246445
0.4862129607657900 0.6820928220952530 0.2245335886334568
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0704111657775863 0.5973100220849277 0.1813167300954814
0.4067407521328002 0.7690716421732895 0.2868921212862293
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9036241819126327 0.5135245424913190 0.1238227942376408
0.7415538696609660 0.6827491209848703 0.2228434922885478
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8209233469097406 0.5977042481336883 0.1811767643599379
0.6576559173067477 0.7674026578826577 0.2846285799150037
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9041145933692609 0.7636904505898527 0.1237857365529996
0.7386644341630334 0.9310655602811418 0.2236747120218405
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8208086791295728 0.8474683233634046 0.1811684085925192
0.6580576226873185 0.5156177207623468 0.2846957600880764
0.8205460000000002 0.5965610000000012 0.0195900000000009
0.6528655504208123 0.7631655100251535 0.1237771927882130
0.9874840216579606 0.9290083873296717 0.2233316585276325

0.736733000000010	0.680055000000030	0.081471999999980
0.5698045117216620	0.8473089212175678	0.1817103874248422
0.9036273760264266	0.5145790642169694	0.2853038740218048
0.820546000000002	0.846561000000012	0.019590000000009
0.6528562848057016	0.5130273390415772	0.1237869873438919
0.9877261060327928	0.6828363148391512	0.2232886870785052
0.736733000000010	0.930055000000030	0.081471999999980
0.5698721675760270	0.5971070845376933	0.1807797831605271
0.9044825333264177	0.7649410490844675	0.2856874279586210
0.4735405598040079	0.5523762912950015	0.3388121891797752
0.4367872765386185	0.5328740054213982	0.3037406631545218
0.2977444950352587	0.4596721450557879	0.3088090330979589
0.403638999999983	0.263308000000021	0.054287000000022
0.2386653625017505	0.4313144514019732	0.1537973148042210
0.0687318320776711	0.0946027858354250	0.2503344927827648
0.403638999999983	0.013308000000021	0.054287000000022
0.2378350924083221	0.1820929031919627	0.1535014516116335
0.0611477451011482	0.3428953373523108	0.2498782278798366
0.153638999999983	0.013308000000021	0.054287000000022
0.4865134161906415	0.1804212805942030	0.1530813444331284
0.3217804875843364	0.3501661047461784	0.2559984747136361
0.153638999999983	0.263308000000021	0.054287000000022

0.4856289916853214	0.4298952038901008	0.1532523233012742
0.3202379097609335	0.0977237371765724	0.2520584810292301
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7363963493994087	0.4300534780429882	0.1526806403964046
0.5702695140321028	0.0974869623585148	0.2517371500840071
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7361933946806519	0.1801139326316346	0.1525671548084846
0.5737321690783350	0.3452829137438745	0.2512200217606163
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9867263474091919	0.1805102508277778	0.1524940404871579
0.8196499947755396	0.3476218133619278	0.2511997489665980
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9868419276862993	0.4301407512919975	0.1525395070886655
0.8192939178063354	0.0967364932736282	0.2512703413313510
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2378704843156355	0.9308106188893120	0.1530462989407878
0.0688786862653261	0.5989973216330396	0.2504231444344461
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.2381224748728776	0.6795139660202962	0.1536389372159890
0.0711421279513663	0.8478791193962579	0.2512324919090556
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.4855815193559057	0.6796536762487158	0.1531904707317146

0.3199583602836264	0.8471104273311265	0.2520250263528395
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.4865495815985383	0.9299856237027175	0.1530611591271961
0.3216863937701405	0.5954880630008483	0.2563188094732464
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7362760847105274	0.9300991436855434	0.1526588361213979
0.5753774110630229	0.5998102123012496	0.2495609918370439
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7368870410806304	0.6803573319170787	0.1524585580264232
0.5736982642966288	0.8532454943445713	0.2510462216881614
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9876215116991226	0.6805519477250153	0.1525314578057023
0.8222767105438842	0.8481836961216507	0.2508583256165204
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9875944266854592	0.9307764152108319	0.1524887140605808
0.8227149943564687	0.5989436435854569	0.2508741024939661

TiH_{1.97}-NOH

10.1930359999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000
0.0000000000000000	0.0000000000000000	27.2903899999999986

H N O Ti

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4043187346087939	0.0137182586913972	0.1237919135900406
0.2334990439065310	0.1773706026039605	0.2228235414204586
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3193793782477417	0.0983387804199566	0.1809614615171868
0.1536478943603971	0.2647929877804742	0.2855726908300631
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4040021986275221	0.2641408160789083	0.1238393567612990
0.2425438973681771	0.4411093053184442	0.2276743703916009
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3196440170378012	0.3478661920935104	0.1809349888630297
0.1522846801818648	0.0154991591066233	0.2855332654893249
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1527940774907639	0.2646308899808447	0.1240475435483061
0.4864612927060295	0.4290440418132280	0.2237072712014517
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0701345863496283	0.3481597890902277	0.1823896737479589
0.3997937279400238	0.0143543939940469	0.2842320661268086
0.3205450000000027	0.3465599999999966	0.0195900000000009

0.1527790080899273 0.0144874081568633 0.1236734098822719
0.4862319886781678 0.1814939940368905 0.2239737279999009
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0693933506231875 0.0978911086473142 0.1813894314201726
0.4019989888409811 0.2639060291157896 0.2852411928977159
0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9019616512548118 0.0139593274930222 0.1239302239760404
0.7363811850125632 0.1810013571726113 0.2248505640854193
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8185946400215846 0.0966368247294370 0.1824465668805551
0.6525093681301211 0.2644677003477641 0.2865438604136004
0.5705460000000002 0.0965599999999966 0.0195900000000009
0.9030791352130894 0.2639943984483454 0.1239669067790859
0.7367954494324013 0.4311054508073026 0.2244833395984399
0.9867330000000010 0.1800550000000030 0.0814719999999980
0.8196127224435603 0.3472283944827874 0.1822605729819884
0.6530386198591139 0.0179236985707878 0.2868109623530489
0.8205460000000002 0.0965599999999966 0.0195900000000009
0.6539897714456538 0.2636792882808904 0.1238552466618244
0.9864078272618799 0.4311625680589966 0.2247001623354035
0.7367330000000010 0.1800539999999984 0.0814719999999980
0.5698394273358534 0.3473402909395011 0.1818156105404887

0.9032711368419363	0.0141617224068807	0.2857198060249672
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6538242133563811	0.0138829663785389	0.1240090481311842
0.9851751982498135	0.1814995168251024	0.2246459329184014
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5698489559177110	0.0973334214378134	0.1820174971795673
0.9031804513017671	0.2644993979673893	0.2856374578487532
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4036585419946971	0.5144647194321396	0.1242329060908638
0.2415479365322721	0.6783350220301562	0.2271890382590624
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3191071880420722	0.5975108200455520	0.1819359273648765
0.1537831325116957	0.7671411550767180	0.2844004373769861
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4034684183122098	0.7636307694575883	0.1241481008183858
0.2315285086801178	0.9363742265536743	0.2218919761881066
0.4867330000000010	0.6800539999999984	0.0814719999999980
0.3189497005965406	0.8477424264807368	0.1791676543402911
0.1439306555630283	0.5111072818606172	0.2864899689096965
0.3205450000000027	0.5965610000000012	0.0195900000000009
0.1534024089740039	0.7631606344037020	0.1239387109921391
0.4887569338305623	0.9305929783321611	0.2246535306364598

0.236733000000010	0.680055000000030	0.081471999999980
0.0690200982286571	0.8481614080860620	0.1810653087400831
0.4070250641161409	0.4929046615658164	0.2849933745979831
0.320545000000027	0.846561000000012	0.019590000000009
0.1528569880378067	0.5131566304486055	0.1240228798186208
0.4805584453594893	0.6770078244852524	0.2247324836566431
0.236733000000010	0.930055000000030	0.081471999999980
0.0696851677840021	0.5973016787918052	0.1819251557165597
0.4007010471808599	0.7952573685322489	0.2807928069034243
0.570546000000002	0.846561000000012	0.019590000000009
0.9035690334232775	0.5134516523244390	0.1239240959260434
0.7381255975282515	0.6815784782032220	0.2239137674073866
0.986733000000010	0.930055000000030	0.081471999999980
0.8196190935139936	0.5972338180204387	0.1818574481734108
0.6709536150458104	0.7685083141573346	0.2816713225085819
0.570546000000002	0.596561000000012	0.019590000000009
0.9029613373333637	0.7634858140877153	0.1238535345099367
0.7323200582853312	0.9284399806831339	0.2258843758915928
0.986733000000010	0.680055000000030	0.081471999999980
0.8195709141967755	0.8472147945681490	0.1808828989394534
0.6537757549570172	0.5138166225560353	0.2865407300787164
0.820546000000002	0.596561000000012	0.019590000000009

0.6524194136274584	0.7631952086077551	0.1243003373555866
0.9910626667705970	0.9344616362144103	0.2228573735084581
0.7367330000000010	0.6800550000000030	0.0814719999999980
0.5683847772843672	0.8462820936716906	0.1838945149053297
0.9033431767760844	0.5154406126516751	0.2859289974232419
0.8205460000000002	0.8465610000000012	0.0195900000000009
0.6535949167796190	0.5133545631143682	0.1238552490669469
0.9857503131752150	0.6815782044578664	0.2239975868701042
0.7367330000000010	0.9300550000000030	0.0814719999999980
0.5692945836411069	0.5972101908368610	0.1820480770636324
0.9032828042086585	0.7653453889978887	0.2856711293553879
0.5391468277869185	0.6680230458927907	0.3361018061847312
0.4913880518591329	0.7080978389527266	0.3173888553340088
0.3602062179967388	0.6396159486007346	0.3341356130301544
0.4036389999999983	0.2633080000000021	0.0542870000000022
0.2366056694764430	0.4318594333604131	0.1535915571456203
0.0692739251984314	0.0985609720510809	0.2511361153716449
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.2363651710805222	0.1812634711483101	0.1522721401210039
0.0706129212799181	0.3483394287079563	0.2517020265951164
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4872450202442697	0.1808521760655666	0.1527234750682050

0.3171189737265362	0.3425611925710178	0.2494145099504576
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.4870380053644247	0.4311943117527254	0.1528794659836364
0.3189247856467474	0.0990820878691270	0.2508267325276127
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7366697341143201	0.4302555918879643	0.1529852000231760
0.5690551823127347	0.0992456234601797	0.2514942773437404
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7363778875639133	0.1802559369990043	0.1532521065874451
0.5699997360734743	0.3468406390682167	0.2516972114846153
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9856956265487672	0.1807775499519730	0.1530358328730852
0.8191903325051626	0.3479764639641307	0.2519160288320385
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9866224301554162	0.4305596351244452	0.1532778997419302
0.8184871070302189	0.0966316859094341	0.2520378564274332
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2359834222851713	0.9315621638556990	0.1518321069958184
0.0689051124714656	0.5992389858219456	0.2510107116637493
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.2364788580010197	0.6788560409066058	0.1533227404424957
0.0686737380714944	0.8485195359741982	0.2509936004907937

0.153638999999983	0.5133080000000021	0.0542870000000022
0.4852781169125612	0.6809512616542602	0.1542678249525873
0.3146031583796102	0.8540509529787285	0.2466285441869978
0.153638999999983	0.7633080000000021	0.0542870000000022
0.4879098094955518	0.9302250272679033	0.1532058786697881
0.3283090809901512	0.6020929406709139	0.2665377258599637
0.903638999999983	0.7633080000000021	0.0542870000000022
0.7350156495403110	0.9298029281144806	0.1535372107635579
0.5716169371307425	0.5949673063070077	0.2513822516194704
0.903638999999983	0.5133080000000021	0.0542870000000022
0.7358377384233319	0.6797128700339039	0.1528659105626770
0.5664368260123770	0.8424027880966564	0.2579863520107669
0.653638999999983	0.5133080000000021	0.0542870000000022
0.9861999745078825	0.6804975677654738	0.1527788281605408
0.8259304614629467	0.8509026650430219	0.2495848425051969
0.653638999999983	0.7633080000000021	0.0542870000000022
0.9858868457952507	0.9311113388652807	0.1523507620179460
0.8200596047068187	0.5980488719202477	0.2517076806708891

TiH_{1.97}-Hv-NH₂O

10.193035999999993	-5.9205420000000002	0.0221310000000000
0.0000000000000000	11.7965890000000009	-0.0158720000000000

0.0000000000000000 0.0000000000000000 27.2903899999999986

H N O Ti

97 1 1 48

Selective dynamics

Direct

0.0705460000000002	0.3465610000000012	0.0195900000000009
0.4028869568671904	0.0131610271447039	0.1239277238721710
0.2346895125225205	0.1787206036332401	0.2245081597347114
0.4867330000000010	0.4300550000000030	0.0814719999999980
0.3189341163067544	0.0966597758111846	0.1820533381733064
0.1472510138850212	0.2615896383301595	0.2855198265035599
0.0705460000000002	0.0965599999999966	0.0195900000000009
0.4032842476942552	0.2640350990168195	0.1241030524377272
0.2345380864406423	0.4293771642306076	0.2249026070554786
0.4867330000000010	0.1800550000000030	0.0814719999999980
0.3187994326949022	0.3467067754265916	0.1823231361198976
0.1512811135437503	0.0127361325761490	0.2863001444100087
0.3205450000000027	0.0965599999999966	0.0195900000000009
0.1532435454368889	0.2634715935865984	0.1239557321848682
0.4863675658807017	0.4319096520552883	0.2258482004570435
0.2367330000000010	0.1800539999999984	0.0814719999999980
0.0682858721698189	0.3462705733536363	0.1813272712373690

0.4016949988606754	0.0133223113031501	0.2861462086918683
0.3205450000000027	0.346559999999966	0.0195900000000009
0.1532350066863560	0.0134320722455595	0.1239833785778067
0.4845541537234230	0.1784874586843808	0.2242441962267771
0.2367330000000010	0.4300550000000030	0.0814719999999980
0.0689993834573611	0.0965932490357681	0.1819092009815541
0.4036207575308065	0.2639943075260527	0.2868385662699550
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.9030873793413076	0.0130036199610876	0.1238227375936036
0.7349184834919270	0.1796046338594300	0.2241908364373485
0.9867330000000010	0.4300550000000030	0.0814719999999980
0.8188027738032444	0.0965573619115198	0.1816640002507098
0.6512677952916639	0.2628105936290038	0.2860409464343007
0.5705460000000002	0.096559999999966	0.0195900000000009
0.9027540333320474	0.2630529375243136	0.1238085757411847
0.7362062264786811	0.4299596533464062	0.2239403945885597
0.9867330000000010	0.1800550000000030	0.0814719999999980
0.8186929451958321	0.3465329013007371	0.1816685850297661
0.6512505137345366	0.0133985548883042	0.2859702793484302
0.8205460000000002	0.096559999999966	0.0195900000000009
0.6527690985180872	0.2631497730828223	0.1238433220680818
0.9840082292125537	0.4305823595634645	0.2238178120577578

0.736733000000010 0.180053999999984 0.081471999999980
0.5690244563893051 0.3468118852428469 0.1816388032628233
0.9010227548671433 0.0128233665050696 0.2858187090657270
0.820546000000002 0.346559999999966 0.019590000000009
0.6527835267273325 0.0130199532802118 0.1238295351031028
0.9841330389735155 0.1777613147759271 0.2238333396147965
0.736733000000010 0.430055000000030 0.081471999999980
0.5686103697000786 0.0965189088275570 0.1817238290224275
0.9001356871992543 0.2625969332805307 0.2862040266655951
0.070546000000002 0.846561000000012 0.019590000000009
0.4029964953488707 0.5132058918701604 0.1240906851684132
0.2343957121942117 0.6802950954548960 0.2244553029768796
0.486733000000010 0.930055000000030 0.081471999999980
0.3188742617603700 0.5965199801870297 0.1822346573424825
0.1511725898560589 0.7632859773637630 0.2863659629296188
0.070546000000002 0.596561000000012 0.019590000000009
0.4032362295498337 0.7627533324573724 0.1240867273545279
0.2358706550736263 0.9300533102073096 0.2245957115097126
0.486733000000010 0.680053999999984 0.081471999999980
0.3189283557834534 0.8465988662711779 0.1820647019946698
0.1472313334295286 0.5107790626639696 0.2854813393581914
0.320545000000027 0.596561000000012 0.019590000000009

0.1531482076551129 0.7631744870144926 0.1240011305653907
0.4844348575973500 0.9305294209402605 0.2241960539024421
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0691817064610285 0.8466406269665498 0.1818679647125848
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1532188524293712 0.5131784827427623 0.1239640667662106
0.4863046450808945 0.6787912919715059 0.2258350285747033
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0688560171715960 0.5966199095951893 0.1819149426932914
0.4037094230200209 0.7644494155008781 0.2867848315887536
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9029641900120174 0.5132907371735679 0.1238352449592769
0.7331026188202037 0.6786858106584411 0.2254336589933004
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8189128204174284 0.5966027636095403 0.1817447833500042
0.6562229210914607 0.7725069309433135 0.2850155895112363
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9026972982345020 0.7630240594155353 0.1240362768319229
0.7364135630076408 0.9306545517059805 0.2238976140300867
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8190102320997203 0.8466196489475892 0.1817188942604211
0.6561340813937628 0.5089419179702523 0.2853220313891729

0.8205460000000002	0.5965610000000012	0.0195900000000009
0.6526222959405016	0.7629373553898620	0.1240537793817624
0.9863805249036558	0.9302861177957091	0.2242476925884091
0.7367330000000010	0.6800550000000030	0.0814719999999980
0.5691434670982699	0.8466298699960357	0.1815173523976414
0.9008463353920427	0.5130350569498170	0.2858748100857346
0.8205460000000002	0.8465610000000012	0.0195900000000009
0.6524858308597630	0.5130589386533231	0.1240699589657777
0.9861264139069355	0.6801808598998255	0.2242521233277179
0.7367330000000010	0.9300550000000030	0.0814719999999980
0.5698347904346882	0.5971152377391699	0.1826597177973200
0.9020379758877194	0.7635082014889325	0.2858726687027186
0.4864368844642198	0.4872530900798273	0.3528575919186631
0.4871953829491714	0.6306739511740215	0.3515441287358008
0.4934025857649471	0.5610819386769548	0.3309187024002972
0.3756311480614251	0.5009076352084215	0.2998321119620477
0.4036389999999983	0.2633080000000021	0.0542870000000022
0.2364265890401732	0.4301353001855485	0.1532957760524994
0.0682405014389730	0.0962390686002505	0.2517268371999152
0.4036389999999983	0.0133080000000021	0.0542870000000022
0.2362678079159272	0.1803167714494335	0.1530299097658153
0.0629763793334588	0.3438807022769366	0.2502860528764591

0.153638999999983 0.013308000000021 0.054287000000022
0.4857945661542478 0.1799140113246954 0.1528286581528479
0.3180140013113145 0.3438922899669245 0.2523468501970033
0.153638999999983 0.263308000000021 0.054287000000022
0.4857962866163720 0.4308912710722862 0.1536755129495064
0.3182404241232244 0.0967767575435708 0.2518832126330688
0.903638999999983 0.263308000000021 0.054287000000022
0.7359788606453214 0.4299302844348655 0.1527586941899222
0.5683635101404767 0.0965494150496082 0.2514497669570890
0.903638999999983 0.013308000000021 0.054287000000022
0.7356420473632207 0.1797578771097486 0.1527278970182385
0.5691466632515778 0.3451088762916557 0.2508193473579515
0.653638999999983 0.013308000000021 0.054287000000022
0.9857599451762786 0.1796540542209632 0.1526753661793014
0.8179690091231955 0.3460242260207725 0.2514656871808549
0.653638999999983 0.263308000000021 0.054287000000022
0.9856957316483644 0.4298446839281619 0.1527126633054350
0.8180167556821222 0.0966198369213904 0.2514326222087772
0.403638999999983 0.763308000000021 0.054287000000022
0.2360750797946163 0.9299585989932980 0.1530076921025570
0.0679577472331881 0.5965945587505144 0.2517347569794150
0.403638999999983 0.513308000000021 0.054287000000022

0.2361586532486989	0.6798354541440990	0.1530508708123393
0.0685146461964170	0.8464410134967021	0.2514942140654599
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.4858944766988272	0.6789313158333803	0.1535827867272778
0.3181401546067239	0.8460656761002703	0.2519375436878821
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.4858144514159841	0.9298566704846281	0.1528549837974949
0.3175012010276623	0.5987200442359789	0.2521977479285480
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7362099175338322	0.9300744682753891	0.1527396199657593
0.5696254829876030	0.5970751477923634	0.2561373523043015
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7352639621895305	0.6795400456421786	0.1531368815507594
0.5692522767967398	0.8490760575125560	0.2506280239175809
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9861056999725777	0.6799175990279936	0.1528655075318691
0.8196239764177793	0.8470912006002489	0.2510718910467201
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9862360479612988	0.9299768363560670	0.1528860875335241
0.8194597991966993	0.5970924335809780	0.2511035071752575

TiH_{1.97}-NH₂O

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H	N	O	Ti
98	1	1	48

Selective dynamics

Direct

0.070546000000002	0.346561000000012	0.019590000000009
0.4037857497406115	0.0138163269243106	0.1237868480733695
0.2340669570934455	0.1773986981232172	0.2232305674558051
0.486733000000010	0.430055000000030	0.081471999999980
0.3194872049316328	0.0975652648236870	0.1812246958149482
0.1533963413974513	0.2640116041102603	0.2852579026254347
0.070546000000002	0.096559999999966	0.019590000000009
0.4038544697387543	0.2641194957180721	0.1238120583818011
0.2445796582277888	0.4444768011347531	0.2290904599463157
0.486733000000010	0.180055000000030	0.081471999999980
0.3199763372761061	0.3477409457099422	0.1811155179373969
0.1523828192361013	0.0146768619691624	0.2858698048195122
0.320545000000027	0.096559999999966	0.019590000000009
0.1539528564938060	0.2652789949442314	0.1241225332363228
0.4867844491187487	0.4288953949386055	0.2236259156016020

0.236733000000010	0.180053999999984	0.081471999999980
0.0710608755374098	0.3483645425159135	0.1820510386973055
0.4015462752750060	0.0151163333715013	0.2849749815677242
0.3205450000000027	0.346559999999966	0.0195900000000009
0.1530592150353019	0.0137887242407628	0.1238276998034554
0.4859981204929016	0.1809041266480295	0.2239373230695739
0.236733000000010	0.4300550000000030	0.081471999999980
0.0693668951231834	0.0971724516404921	0.1815359968328954
0.4019142656592675	0.2632124089614457	0.2851282175688003
0.5705460000000002	0.3465610000000012	0.0195900000000009
0.9032523139988234	0.0140765095144675	0.1239076358664563
0.7368494552765616	0.1813892761110201	0.2244509259031480
0.986733000000010	0.4300550000000030	0.081471999999980
0.8197418911755789	0.0975605323588341	0.1818234076325086
0.6534771414091843	0.2648578905593745	0.2867750652641238
0.5705460000000002	0.096559999999966	0.0195900000000009
0.9039124113039138	0.2643776531010512	0.1239236031570540
0.7369272331751472	0.4311899385199644	0.2243904742446208
0.986733000000010	0.1800550000000030	0.081471999999980
0.8202720714209684	0.3476923288195639	0.1819798500669604
0.6531562229217431	0.0159819754430564	0.2864422216071826
0.8205460000000002	0.096559999999966	0.0195900000000009

0.6537575832640424	0.2638975209901946	0.1237838576910324
0.9868518220495851	0.4313966526383842	0.2244050886482854
0.7367330000000010	0.1800539999999984	0.0814719999999980
0.5701815449852936	0.3472236399142185	0.1817596970065710
0.9028632240612690	0.0146398066210533	0.2860853707711685
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6540867912724913	0.0143140952750412	0.1238679155692162
0.9859151460872490	0.1804242824502079	0.2242533663610359
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5701558805069441	0.0980987901481349	0.1817514126969352
0.9034463540058889	0.2645577596699750	0.2854551896452546
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4040533093292626	0.5141338281592751	0.1240992818234396
0.2442090021567218	0.6763100746630538	0.2288332308539306
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3212455298817627	0.5983364258452278	0.1819463210980289
0.1536206156014166	0.7663643556953373	0.2851048139189792
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4041049721920025	0.7641535663286667	0.1240485647922976
0.2336803554726477	0.9330644987764081	0.2229819034612018
0.4867330000000010	0.6800539999999984	0.0814719999999980
0.3198675306173915	0.8477020650949689	0.1807938642037616

0.1384216556459477 0.5079920843925776 0.2854312838300271
0.3205450000000027 0.5965610000000012 0.0195900000000009
0.1540599593976755 0.7629636317373771 0.1241166648120831
0.4868561009277872 0.9334745435078937 0.2235581727099124
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0693173047805931 0.8477264279575506 0.1815259892026467
0.4098730314703548 0.4940719011518541 0.2855001267001323
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1538752662210343 0.5139555130607075 0.1241773659731121
0.4773566878561474 0.6764626018515829 0.2291289618311831
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0709885889174460 0.5979994293224645 0.1819042419067852
0.4083462316913957 0.7930509683693249 0.2847984038283984
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9039771596223736 0.5136572554689982 0.1239379493361221
0.7382004852649996 0.6818796457811834 0.2240449616567665
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8199293437817147 0.5974380592254536 0.1817741858805887
0.6577708151874847 0.7667288363772301 0.2840645941299074
0.5705460000000002 0.5965610000000012 0.0195900000000009
0.9033022150006759 0.7634363200659733 0.1239389461808683
0.7376088684794948 0.9314584263909863 0.2241383327184485

0.986733000000010 0.680055000000030 0.081471999999980
0.8196774199362868 0.8474307735251123 0.1817279831380027
0.6536375249908338 0.5138906916741613 0.2862936884476808
0.820546000000002 0.596561000000012 0.019590000000009
0.6531609268904464 0.7635816858276080 0.1241276170519589
0.9869802062073962 0.9314219446037643 0.2237788349743402
0.736733000000010 0.680055000000030 0.081471999999980
0.5691538374240713 0.8470749130635278 0.1821556852094628
0.9036186072576853 0.5154332305110304 0.2854718290341510
0.820546000000002 0.846561000000012 0.019590000000009
0.6539977935675287 0.5137534385542195 0.1238811004973830
0.9860611688296289 0.6817543917410823 0.2240541462057026
0.736733000000010 0.930055000000030 0.081471999999980
0.5692450033201147 0.5973781898494589 0.1819690050852790
0.9029661181089570 0.7647543260489950 0.2861578649418982
0.4882569490911449 0.6152422126518003 0.3539182096558522
0.4850032843251276 0.7575926344369631 0.3536197945422269
0.4484199217383620 0.6662947653027799 0.3379581499183151
0.3108218628862570 0.5951098992999627 0.3418485986868721
0.403638999999983 0.263308000000021 0.054287000000022
0.2381529092171540 0.4330357918689240 0.1539034948388303
0.0687407723878243 0.0969537902123291 0.2512394178160530

0.403638999999983	0.013308000000021	0.054287000000022
0.2365138378818036	0.1808118258902323	0.1524509619903737
0.0703983819775305	0.3471422381839214	0.2510501767733608
0.153638999999983	0.013308000000021	0.054287000000022
0.4869780639767100	0.1807917028006952	0.1526933270738381
0.3176853901178357	0.3430252076747904	0.2495740505094715
0.153638999999983	0.263308000000021	0.054287000000022
0.4874001324275045	0.4311354423977208	0.1528864960145115
0.3190835305458181	0.0977391411755702	0.2509674587148484
0.903638999999983	0.263308000000021	0.054287000000022
0.7369285684646615	0.4302555395308485	0.1528786921187360
0.5700007792321986	0.0998435074489381	0.2515576108585574
0.903638999999983	0.013308000000021	0.054287000000022
0.7368842680487654	0.1812236124383236	0.1528759094824860
0.5702324524389368	0.3463204475651419	0.2516264444365361
0.653638999999983	0.013308000000021	0.054287000000022
0.9866013141039540	0.1808840623094770	0.1528634083658866
0.8192361526299827	0.3476870221614103	0.2515857649283350
0.653638999999983	0.263308000000021	0.054287000000022
0.9876257809018896	0.4310685057534694	0.1531824078719108
0.8194139413855498	0.0974507394969142	0.2515950116686440
0.403638999999983	0.763308000000021	0.054287000000022

0.2363324139763085 0.9307094012667163 0.1523760253034171
0.0699827984660852 0.5998222570482458 0.2508217288206648
0.4036389999999983 0.5133080000000021 0.0542870000000022
0.2382616867410899 0.6798663735778330 0.1538199658611664
0.0688600551920115 0.8482727015292619 0.2513008486164396
0.1536389999999983 0.5133080000000021 0.0542870000000022
0.4856220283635751 0.6803369971768177 0.1536171781850644
0.3172204681147704 0.8514822987677966 0.2491279545912015
0.1536389999999983 0.7633080000000021 0.0542870000000022
0.4875713916420264 0.9309693866882925 0.1528213483659240
0.3249454931358916 0.6010617669832177 0.2715156482304805
0.9036389999999983 0.7633080000000021 0.0542870000000022
0.7363065284479302 0.9305530328162508 0.1529696308864495
0.5724558267371834 0.5951306324150865 0.2509890993194828
0.9036389999999983 0.5133080000000021 0.0542870000000022
0.7364290021228235 0.6803705891994467 0.1529603149423953
0.5717293427885952 0.8527033400115945 0.2513456932448180
0.6536389999999983 0.5133080000000021 0.0542870000000022
0.9866841002740800 0.6805607447922908 0.1528469757716817
0.8210688791841809 0.8484965701640215 0.2513428280246811
0.6536389999999983 0.7633080000000021 0.0542870000000022
0.9859607987145043 0.9304581219921102 0.1527403175449379

0.8199450349708958 0.5981377661155022 0.2515461692616158

TiH_{1.97}-Hv-O

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H	O	Ti
95	1	48

Selective dynamics

Direct

0.070546000000002	0.346561000000012	0.019590000000009
0.4037302553397504	0.0134585939459664	0.1239263242275081
0.2366078612425869	0.1791591944395959	0.2251415050202408
0.486733000000010	0.430055000000030	0.081471999999980
0.3201980126393187	0.0970237697210753	0.1821998387878044
0.1506317981426998	0.2630790235704218	0.2854222467001886
0.070546000000002	0.096559999999966	0.019590000000009
0.4037941704845837	0.2636522368038990	0.1240197341740991
0.2345260292634816	0.4292341213535067	0.2239129082436122
0.486733000000010	0.180055000000030	0.081471999999980
0.3199293046177997	0.3468714020590125	0.1818573709743308
0.1532620751752521	0.0134833518514661	0.2865561452894522

0.3205450000000027 0.0965599999999966 0.0195900000000009
0.1540408901938768 0.2635015157517918 0.1239978187984677
0.4885010155454968 0.4293089152301630 0.2239565917236948
0.2367330000000010 0.1800539999999984 0.0814719999999980
0.0697753610369014 0.3469285837143614 0.1814089353221478
0.4041400981629806 0.0143381019713890 0.2861983090892480
0.3205450000000027 0.3465599999999966 0.0195900000000009
0.1539838123597561 0.0135976035479370 0.1240464809751098
0.4863543370584887 0.1790304110771390 0.2242491475382992
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0702091374882275 0.0969997856736544 0.1821306350371380
0.4051916163370379 0.2632192994471978 0.2855355088465215
0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9040897628570400 0.0134401807646792 0.1239041493510039
0.7372412107819110 0.1806780257956357 0.2241682718415945
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8202676197857990 0.0971303798652829 0.1817687875746148
0.6541135721084568 0.2636993753952581 0.2861123062103495
0.5705460000000002 0.0965599999999966 0.0195900000000009
0.9040127179528286 0.2636123545494897 0.1238666231253981
0.7389500457362426 0.4316114597290741 0.2242130722575165
0.9867330000000010 0.1800550000000030 0.0814719999999980

0.8201800000418050 0.3471793928672822 0.1817059435447619
0.6538398674650422 0.0149048045769433 0.2861720872630610
0.8205460000000002 0.0965599999999966 0.0195900000000009
0.6538551140895180 0.2636932121083205 0.1238990844526331
0.9865766791541699 0.4317777523435701 0.2241928268350931
0.7367330000000010 0.1800539999999984 0.0814719999999980
0.5704283261237798 0.3470216372446377 0.1814588039539057
0.9033288163330306 0.0144657351334003 0.2860817167682468
0.8205460000000002 0.3465599999999966 0.0195900000000009
0.6538912170400640 0.0134427987993515 0.1238736971807617
0.9865092121570794 0.1788708074510062 0.2242671259492265
0.7367330000000010 0.4300550000000030 0.0814719999999980
0.5702181642850482 0.0972104355103373 0.1817328677196695
0.9026876667701743 0.2638310025830260 0.2861549894532919
0.0705460000000002 0.8465610000000012 0.0195900000000009
0.4038537901991403 0.5135711471075609 0.1239619915694157
0.2364907520101402 0.6813350326995886 0.2250832759938596
0.4867330000000010 0.9300550000000030 0.0814719999999980
0.3200802527047459 0.5972230529391627 0.1818542788382987
0.1532142458764887 0.7645436292796646 0.2866139489043591
0.0705460000000002 0.5965610000000012 0.0195900000000009
0.4037341101303922 0.7634416097042722 0.1240008827720143

0.2374647178740343 0.9307181763232769 0.2246271736103824
0.4867330000000010 0.6800539999999984 0.0814719999999980
0.3202249416146800 0.8472963403867734 0.1822101300633701
0.1506233021644570 0.5124741819901067 0.2854325473548214
0.3205450000000027 0.5965610000000012 0.0195900000000009
0.1540011635548857 0.7635713007146478 0.1240621467323737
0.4862232729155858 0.9313850789029021 0.2241922698148285
0.2367330000000010 0.6800550000000030 0.0814719999999980
0.0703401838333681 0.8471801561201604 0.1821250704120888
0.3205450000000027 0.8465610000000012 0.0195900000000009
0.1540687603176936 0.5137945375183014 0.1239994661588368
0.4885373478114635 0.6832049796945976 0.2239044420615972
0.2367330000000010 0.9300550000000030 0.0814719999999980
0.0701309787557364 0.5972579201796949 0.1821364432047748
0.4052296685206641 0.7666497059665370 0.2854827617243223
0.5705460000000002 0.8465610000000012 0.0195900000000009
0.9040693653626624 0.5138107779935537 0.1239122009692282
0.7392170334634576 0.6815242141563597 0.2249881646976969
0.9867330000000010 0.9300550000000030 0.0814719999999980
0.8205176050961170 0.5972962824686814 0.1821685793654557
0.6545125608854366 0.7668517889230464 0.2854036314868995
0.5705460000000002 0.5965610000000012 0.0195900000000009

0.9040526802776332	0.7636289322407673	0.1240455334562508
0.7390480316579299	0.9314454680688651	0.2242201920953813
0.986733000000010	0.680055000000030	0.081471999999980
0.8204878440957992	0.8472652339926561	0.1821735446283174
0.6547967649470032	0.5126260303885727	0.2854587232365911
0.820546000000002	0.596561000000012	0.019590000000009
0.6539645781396639	0.7634237773869808	0.1240049990739965
0.9872640001425917	0.9303722803222120	0.2246139823032585
0.736733000000010	0.680055000000030	0.081471999999980
0.5704935495059428	0.8476019252058081	0.1813919337539354
0.9033999872685368	0.5135974518716542	0.2861016960259652
0.820546000000002	0.846561000000012	0.019590000000009
0.6537995291649095	0.5137064776388368	0.1240239435771104
0.9872941795881288	0.6809366037411431	0.2245359109162367
0.736733000000010	0.930055000000030	0.081471999999980
0.5706607331507951	0.5974772016571053	0.1817228100339952
0.9043097663557447	0.7645304044622628	0.2864939733460000
0.4038180545991557	0.5145545258613813	0.2890003515466973
0.403638999999983	0.263308000000021	0.054287000000022
0.2374985396841431	0.4305767113224549	0.1531141676025178
0.0706747731239405	0.0969102094087454	0.2518841138899865
0.403638999999983	0.013308000000021	0.054287000000022

0.2371542178288828	0.1803889438348775	0.1532612446641103
0.0664054230682377	0.3455180077990055	0.2505655003578076
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4869003880042755	0.1801642643620991	0.1528750065614154
0.3212748623881070	0.3489121958536804	0.2523123654818380
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.4866452995061128	0.4306995485486427	0.1531996601136517
0.3197944212825042	0.0969380142857552	0.2519079250900826
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7372750136647215	0.4305929992283953	0.1528660000441083
0.5705156258840998	0.0973913385247497	0.2514627071614414
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7371012566340186	0.1803598110656451	0.1526897398536012
0.5723312402865265	0.3456050897349813	0.2507112899882896
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9870195629310812	0.1800980458000132	0.1528637790505125
0.8204169415650935	0.3472555201938490	0.2514147778441012
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9869662184286757	0.4304692939164971	0.1528699493700232
0.8202951821699902	0.0975726435255437	0.2515288151297638
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2371875267333171	0.9304333893199829	0.1531259999959130

0.0706624913754960	0.5983448090351734	0.2518797069799297
0.4036389999999983	0.5133080000000021	0.0542870000000022
0.2371209131051613	0.6803657792853975	0.1533530102847791
0.0705575087222580	0.8474209811577676	0.2517942492841105
0.1536389999999983	0.5133080000000021	0.0542870000000022
0.4867755029673987	0.6798430352506719	0.1530978423552113
0.3196679016262100	0.8470680745541769	0.2519413497515064
0.1536389999999983	0.7633080000000021	0.0542870000000022
0.4869972957848602	0.9305089917758586	0.1528921096011800
0.3211404520624276	0.5966365317734448	0.2523278610164055
0.9036389999999983	0.7633080000000021	0.0542870000000022
0.7373584928712205	0.9303992547509606	0.1528763181628639
0.5692511100648719	0.5966721503928014	0.2521025454695187
0.9036389999999983	0.5133080000000021	0.0542870000000022
0.7372155572409341	0.6804155728678422	0.1532156692041273
0.5723061128836855	0.8513327578009694	0.2505659142892185
0.6536389999999983	0.5133080000000021	0.0542870000000022
0.9871073558302867	0.6803805896277025	0.1530945377691691
0.8208852509828048	0.8471780272219982	0.2518906749090953
0.6536389999999983	0.7633080000000021	0.0542870000000022
0.9871298444616269	0.9303542521771784	0.1531282222972594
0.8211400404088105	0.5981617138845264	0.2518659522293635

TiH_{1.97}-O

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H	O	Ti
96	1	48

Selective dynamics

Direct

0.070546000000002	0.346561000000012	0.019590000000009
0.4048046723839692	0.0141218252806962	0.1238548478822203
0.2333896254451660	0.1743145349666602	0.2222877145569577
0.486733000000010	0.430055000000030	0.081471999999980
0.3198813362689878	0.0976958741508702	0.1810571531968795
0.1535489975776624	0.2634193402073619	0.2852057886387446
0.070546000000002	0.096559999999966	0.019590000000009
0.4048311640608910	0.2649992334351564	0.1238768758816523
0.2393406901237995	0.4354778662591817	0.2255500171016991
0.486733000000010	0.180055000000030	0.081471999999980
0.3197002021973332	0.3476186729972937	0.1802433596496302
0.1528745513443850	0.0150523687120028	0.2854193097353241
0.320545000000027	0.096559999999966	0.019590000000009

0.1535130998026745 0.2649705241979847 0.1238631315374773
0.4883369589464458 0.4354973196502051 0.2253927416472435
0.2367330000000010 0.1800539999999984 0.0814719999999980
0.0701673987434007 0.3482321597638379 0.1823350480918853
0.4012476267929058 0.0142146839639674 0.2852356630394860
0.3205450000000027 0.3465599999999966 0.0195900000000009
0.1536359461079934 0.0140025306965502 0.1236777378924684
0.4873132785099031 0.1819401056942583 0.2242642465179633
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0698822519185823 0.0977165714343168 0.1809271319318323
0.4011359484948823 0.2637763364207720 0.2853174583216757
0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9027253902837319 0.0141906943530183 0.1238624760104867
0.7365735069896671 0.1810924579796028 0.2248996327270567
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8194041702207976 0.0974829522752651 0.1822584993913822
0.6521071764127552 0.2643723889474314 0.2860938337394209
0.5705460000000002 0.0965599999999966 0.0195900000000009
0.9032930455722007 0.2644037447508291 0.1239418637356330
0.7365182791878297 0.4316795489873541 0.2249681479361150
0.9867330000000010 0.1800550000000030 0.0814719999999980
0.8198147708217248 0.3477906197082878 0.1824352874442134

0.6532272724447643	0.0161091761510464	0.2863041918586727
0.8205460000000002	0.0965599999999966	0.0195900000000009
0.6543973923864960	0.2644566892797812	0.1239651803543587
0.9871948894026883	0.4316473073404075	0.2249878774811571
0.7367330000000010	0.1800539999999984	0.0814719999999980
0.5698634144125706	0.3482167141151197	0.1822638623154493
0.9042357696456925	0.0142980859029734	0.2851244660824133
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6539400733770355	0.0144873718763727	0.1239357869718117
0.9863354740594752	0.1818431756119801	0.2243541732123321
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5700347046914093	0.0974019345568102	0.1821057733436470
0.9033699822336161	0.2644661234344420	0.2861483887693031
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4038008775880880	0.5146076427076748	0.1241470648601676
0.239278880919610	0.6799119820990943	0.2254076419393412
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3199266988469583	0.5977376108018977	0.1837912117784829
0.1537998226937699	0.7669207866469254	0.2852535997625840
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4039247967340894	0.7636608464629344	0.1240789396896054
0.2330965445073440	0.9350170351842380	0.2221884807392193

0.486733000000010 0.680053999999984 0.081471999999980
0.3198754105434549 0.8476856519068448 0.1801060677318031
0.1518758841963173 0.5146949042283169 0.2863766904784816
0.320545000000027 0.596561000000012 0.019590000000009
0.1535208956020177 0.7627989425406877 0.1238651081408578
0.4882847977783940 0.9289209848217970 0.2253259667979479
0.236733000000010 0.680055000000030 0.081471999999980
0.0698891503226358 0.8477093701180550 0.1810654124822295
0.3879892801641755 0.4828535493841900 0.2850454964733516
0.320545000000027 0.846561000000012 0.019590000000009
0.1531420573876582 0.5136817091040826 0.1239551840735519
0.4864933743733905 0.6815924421555069 0.2203416709608689
0.236733000000010 0.930055000000030 0.081471999999980
0.0702248764433580 0.5975812344938540 0.1821832554271608
0.3869776689118238 0.7812917497891760 0.2849537744148626
0.570546000000002 0.846561000000012 0.019590000000009
0.9031900620327385 0.5132174151186608 0.1239774612987818
0.7325067950037559 0.6797745725276230 0.2253861052650498
0.986733000000010 0.930055000000030 0.081471999999980
0.8193820620997490 0.5977227584113212 0.1822680012429493
0.6849587008452669 0.7805338131794112 0.2850027835379088
0.570546000000002 0.596561000000012 0.019590000000009

0.9026355854025723 0.7627643477512367 0.1238887834861547
0.7324414204505307 0.9288413078842980 0.2254323908755410
0.9867330000000010 0.6800550000000030 0.0814719999999980
0.8198983901139928 0.8478349804127804 0.1801965433617051
0.6532300596866495 0.5146718392277492 0.2864093415002483
0.8205460000000002 0.5965610000000012 0.0195900000000009
0.6530108794156444 0.7637934094204503 0.1241467651790050
0.9936730974927833 0.9346885838721163 0.2222722365375069
0.7367330000000010 0.6800550000000030 0.0814719999999980
0.5698352479373034 0.8476875331085942 0.1837621724066289
0.9035355792662412 0.5159273332401404 0.2861043321879456
0.8205460000000002 0.8465610000000012 0.0195900000000009
0.6536901853861478 0.5138892711485270 0.1240008150229589
0.9862284014493975 0.6808585711060644 0.2242970714579594
0.7367330000000010 0.9300550000000030 0.0814719999999980
0.5696650828446523 0.5978738859690027 0.1837227690952988
0.9039681856666062 0.7669125490240376 0.2852509576822334
0.4860511256723462 0.6816621384063278 0.2992766502904310
0.4036389999999983 0.2633080000000021 0.0542870000000022
0.2367803482684234 0.4322371005266094 0.1533116120091052
0.0699434896782264 0.0979840756419674 0.2507215101490824
0.4036389999999983 0.0133080000000021 0.0542870000000022

0.2368815054872336	0.1809609070914119	0.1520607435179784
0.0702046758799695	0.3477467896317019	0.2518562106650685
0.1536389999999983	0.0133080000000021	0.0542870000000022
0.4876641165703722	0.1812916997452050	0.1528551544835492
0.3158425421545069	0.3400675176185865	0.2483359010452819
0.1536389999999983	0.2633080000000021	0.0542870000000022
0.4876902118825124	0.4322559303884258	0.1533221567778697
0.3197437238310816	0.0979928050998889	0.2509969602468362
0.9036389999999983	0.2633080000000021	0.0542870000000022
0.7365375606457388	0.4310837998918154	0.1533858066437302
0.5689686489357070	0.0981971472060521	0.2515509980666978
0.9036389999999983	0.0133080000000021	0.0542870000000022
0.7367571202366431	0.1807650861769425	0.1532995816745656
0.5690613980090993	0.3476399044938097	0.2518276641575937
0.6536389999999983	0.0133080000000021	0.0542870000000022
0.9863083560057772	0.1814177918938584	0.1528196850725117
0.8198428392370062	0.3482699425514773	0.2520113342605825
0.6536389999999983	0.2633080000000021	0.0542870000000022
0.9868758546322141	0.4308859661145665	0.1533329357679327
0.8201875405440316	0.0978621279416844	0.2517752337510984
0.4036389999999983	0.7633080000000021	0.0542870000000022
0.2367830337536410	0.9308136603333416	0.1520549591912230

0.0699252061271550	0.5992181903716032	0.2516191660681639
0.403638999999983	0.513308000000021	0.054287000000022
0.2369961835001954	0.6794873577308866	0.1532332407304005
0.0700070814835726	0.848373651789967	0.2509904703344623
0.153638999999983	0.513308000000021	0.054287000000022
0.4867228961019823	0.6809437055443746	0.1540285902086641
0.3157344667222319	0.8524044092342834	0.2481909574410935
0.153638999999983	0.763308000000021	0.054287000000022
0.4880790186546419	0.9305949279364759	0.1532056126325473
0.3282787866583544	0.6024544006006384	0.2576053453357935
0.903638999999983	0.763308000000021	0.054287000000022
0.7354025263935628	0.9308433153270995	0.1532770546635272
0.5652026789322652	0.6026844972043025	0.2573810601005491
0.903638999999983	0.513308000000021	0.054287000000022
0.7353304600930111	0.6798537130571456	0.1533154485629832
0.5654343661791904	0.8397189123422114	0.2575410578068817
0.653638999999983	0.513308000000021	0.054287000000022
0.9863477091667757	0.6799226990637027	0.1528762000189719
0.8277999273896923	0.8522476896534501	0.2482286545712685
0.653638999999983	0.763308000000021	0.054287000000022
0.9866783396704600	0.9307370816873097	0.1520591306491577
0.8203688206974453	0.5990556138172524	0.2518266098439289

TiH_{1.97}-Hv-OH

10.193035999999993	-5.920542000000002	0.022131000000000
0.000000000000000	11.796589000000009	-0.015872000000000
0.000000000000000	0.000000000000000	27.290389999999986

H	O	Ti
96	1	48

Selective dynamics

Direct

0.070546000000002	0.346561000000012	0.019590000000009
0.4036842359938647	0.0135139807080544	0.1239132137484811
0.2372091969480619	0.1804137999416050	0.2246466088690448
0.486733000000010	0.430055000000030	0.081471999999980
0.3202329758239590	0.0972367049110316	0.1821868501160681
0.1520329911996298	0.2647227974539496	0.2863383269376881
0.070546000000002	0.096559999999966	0.019590000000009
0.4040319210828985	0.2640710634439066	0.1239492349613837
0.2367548938009637	0.4305052405410452	0.2247862264663757
0.486733000000010	0.180055000000030	0.081471999999980
0.3204761642204682	0.3476129640387655	0.1823702561846521
0.1535182079646808	0.0139977327676079	0.2866214821111965
0.320545000000027	0.096559999999966	0.019590000000009

0.1542610490770645 0.2639507009834872 0.1239412002215308
0.4875511243215874 0.4304140837747400 0.2248273727196848
0.2367330000000010 0.1800539999999984 0.0814719999999980
0.0700805875029838 0.3471677987214514 0.1815039533193286
0.4042978456405955 0.0146731627829320 0.2861415058464953
0.3205450000000027 0.3465599999999966 0.0195900000000009
0.1541178096277359 0.0139606884793279 0.1240418978228749
0.4865328491529735 0.1794955888499371 0.2242010562875232
0.2367330000000010 0.4300550000000030 0.0814719999999980
0.0703743253116762 0.0972496425818189 0.1821848259566229
0.4055105550870017 0.2645763779817811 0.2863758997251439
0.5705460000000002 0.3465610000000012 0.0195900000000009
0.9040990618256416 0.0135522322066789 0.1238968171190542
0.7375297723686974 0.1809389116618868 0.2241298494262737
0.9867330000000010 0.4300550000000030 0.0814719999999980
0.8204171124372153 0.0973079382969460 0.1818007182209306
0.6540719348109472 0.2639118857087752 0.2861937068510804
0.5705460000000002 0.0965599999999966 0.0195900000000009
0.9041339882043495 0.2637881369386140 0.1238506622014286
0.7387609241238913 0.4316956685916878 0.2242342736639265
0.9867330000000010 0.1800550000000030 0.0814719999999980
0.8203723951861936 0.3473678705560048 0.1817948225576501

0.6540074105215260	0.0150696944744799	0.2862243659531501
0.8205460000000002	0.0965599999999966	0.0195900000000009
0.6538467491817191	0.2637243406195049	0.1238572043962069
0.9869005744665970	0.4317466179973479	0.2241481676403745
0.7367330000000010	0.1800539999999984	0.0814719999999980
0.5705082998343788	0.3471371459254025	0.1815779488758127
0.9034421363122160	0.0144959254932486	0.2862135228632265
0.8205460000000002	0.3465599999999966	0.0195900000000009
0.6538422346929537	0.0135325535398628	0.1238473576961509
0.9868871255201392	0.1794677124951175	0.2241604320163831
0.7367330000000010	0.4300550000000030	0.0814719999999980
0.5702424645520312	0.0973059794882218	0.1817404169385261
0.9030451028565080	0.2640403873907463	0.2863417398717563
0.0705460000000002	0.8465610000000012	0.0195900000000009
0.4040964861503774	0.5137286464382704	0.1239406989035466
0.2371601612389763	0.6810883032831748	0.2246524057317729
0.4867330000000010	0.9300550000000030	0.0814719999999980
0.3205794000340543	0.5971451231174628	0.1823691467150196
0.1534360912632808	0.7645806635643596	0.2866331366915754
0.0705460000000002	0.5965610000000012	0.0195900000000009
0.4039972007310303	0.7634055865225046	0.1239452379761198
0.2375626400854782	0.9309226962931494	0.2246691459627441

0.486733000000010	0.680053999999984	0.081471999999980
0.3202166197614549	0.8472686942857475	0.1822247281441884
0.1520120893127092	0.5124173866127504	0.2863022281975043
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TiH_{1.97}-OH

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H	O	Ti
97	1	48

Selective dynamics

Direct

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